The Future of U.S. Chemistry Research: Benchmarks and Challenges
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THE FUTURE OF U.S. Chemistry Research

BENCHMARKS AND CHALLENGES

Committee on Benchmarking the Research Competitiveness
of the United States in Chemistry

Board on Chemical Sciences and Technology

Division on Earth and Life Studies

NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES

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Acknowledgment of Reviewers

This report has been reviewed in draft form by persons chosen for their diverse perspectives and technical expertise in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making the published report as sound as possible and to ensure that it meets institutional standards of 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:

Dr. Andreas Manz, ISAS—Institute for Analytical Sciences, Dortmund, Germany
Dr. John M. Campbell, Sr., (Retired President and CEO, Campbell Companies), Norman, OK
Dr. Catherine E. Costello, Boston University School of Medicine, Boston, MA
Dr. Miles P. Drake, Weyerhaeuser Company, Allentown, PA
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Although the reviewers listed above provided many constructive comments and suggestions, they did not see the final draft of the report before its release. The review was overseen by Dr. Maxine Savitz, retired, General Manager, Technology/Partnerships Honeywell Inc, appointed by the National Research Council and Dr. C. Bradley Moore, Northwestern University, appointed by the Division on Earth and Life Studies, who 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 authors and the institution.

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Summary

WHY BENCHMARK THE RESEARCH COMPETITIVENESS OF U.S. CHEMISTRY NOW?

The American people, Congress, and the President have growing concerns about U.S. competitiveness and this country's ability to lead the world in innovation and job creation. A recent National Research Council report, *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, evaluated the present status of U.S. competitiveness and made specific recommendations for improvements.

In addition to concerns about overall U.S. competitiveness, there are compelling reasons to assess the standing of U.S. chemistry now. The field of chemistry is currently facing major issues of identity and purpose in a time when it is expanding beyond its traditional core toward areas related to biology, materials science, and nanotechnology. Chemistry is facing a crucial time of change and is struggling to position itself to meet the needs of the future. However, before addressing questions of how U.S. chemistry must shift to address future needs, it is imperative to understand its current health and international standing.

THE PANEL AND ITS CHARGE

At the request of the Department of Energy Basic Energy Sciences Chemical Sciences, Geosciences, and Biosciences Division, and the National Science Foundation Chemistry Division, the National Academies' Board on

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Chemical Sciences and Technology performed an international benchmarking exercise to determine the standing of the U.S. research enterprise in the field of chemistry relative to its international peers.

The field of chemistry was benchmarked by an ad hoc panel of 13 members, 12 from the United States and one from Switzerland, with expertise across the 11 selected areas covered in the report, which are analytical, atmospheric, biological, chemical education, inorganic, macromolecules, materials and nanoscience, nuclear/radiochemistry, organic, physical, and theory/computation. The panel was charged with addressing three questions:

1. What is the current position of U.S. chemistry relative to that of other regions or countries?
2. What key factors influence U.S. performance in chemistry?
3. On the basis of current trends in the United States and abroad, what will be the relative U.S. position in the near term and in the longer term?

Following a process similar to that established in *Experiments in International Benchmarking of U.S. Research Fields*,[1] the panel was instructed to perform their charge in a short time frame and with a limited budget. The group met one time in person, and otherwise met via teleconference. Thus, in order to adequately respond to their charge, the panel had to limit the scope of the benchmarking exercise to assessing the state of basic (fundamental) chemistry research as determined by the open published literature, the opinions of their peers, and other sources of easily accessible information. This benchmarking exercise was conducted based on the premise that evaluating this type of more "academic" research information would give a good estimate of the quality and quantity of fundamental research being conducted, which could in turn be used as an indicator of competitiveness of the larger chemical enterprise. However, this exercise in no way presents a complete picture of the level of research activity of the enterprise—particularly the industrial component.

The quantitative and qualitative measures employed to compare U.S. chemistry with that in other nations included analysis of journal publications (numbers of papers, citations of papers, most cited papers, most cited authors, most accessed papers), largely derived from Thompson ISI Essential Science Indicators, as well as data provided by the American Chemical Society Publications Division. In addition, the panel asked leading experts

[1] Committee on Science, Engineering, and Public Policy, 2000, *Experiments in International Benchmarking of U.S. Research Fields*, National Academy Press, Washington, D.C.

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from the United States and abroad to identify the "best of the best" whom they would invite to an international conference in their subfield. The national makeup of these "virtual world congresses" provided qualitative information on leadership in chemistry. International prizes and congresses were also considered. The panel steered clear of distinguishing between academic, industrial, and governmental laboratory research performers; all of whom were considered in the exercise. Finally, the panel examined trends in the numbers of degrees, employment, and research funding of U.S. chemistry, relying heavily upon the NSF S&E Indicators 2006 and earlier years.

The resulting report details the status of U.S. competitiveness of research in chemistry and its subareas. This benchmarking exercise attempts to determine the current status of the discipline and to extrapolate the future status based on current trends. The report does not make judgments about the relative importance of leadership in each area or make recommendations on actions to be taken to ensure such leadership in the future.

WHAT IS CHEMISTRY RESEARCH?

Chemists view the world at the atomic and molecular levels. They relate the properties of all substances to the detailed composition and atomic arrangements of all the chemical components. Understanding how the properties and reactivity of substances are related to their molecular structures helps chemists design new molecules with desirable properties and allows them to invent *new* transformations to synthesize and manufacture the new substances. Chemists seek to discover the components of the chemical universe—from molecules to organized chemical systems, such as living cells and whole organisms—and to understand how these components interact and change. Synthetic chemists create and characterize new molecules and materials unknown in the natural world and develop the novel transformations needed to make them. Chemical scientists produce tangible benefits to society when they design and engineer useful substances, such as new pharmaceuticals and polymeric materials.

HOW IMPORTANT IS IT FOR THE UNITED STATES TO LEAD IN CHEMISTRY RESEARCH?

Chemistry is both a central science and an enabling science. Chemistry plays a key role in conquering diseases, solving energy problems, ameliorating environmental problems, providing the discoveries that lead to new industries, and developing new materials for national defense and new technologies for homeland security.

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KEY FINDINGS AND CONCLUSIONS

Today, chemistry research in the United States is stronger than in any other single country, but competition from Europe and Asia is rapidly increasing.

Evidence for current, but eroding, U.S. leadership in chemistry comes from analysis of publications, citations, highly cited papers and highly cited chemists, virtual congresses, and scientific awards.

In 2003 the United States published about 19 percent of the world's chemistry papers, down from 23 percent in 1988. While the U.S. published a larger percentage of papers than any other single nation, this is about four percent less than the number of papers published in Western Europe. Although U.S. chemists have been publishing at a steady rate of about 15,000 chemistry papers per year, chemists from other nations are increasing their rate of publication, as determined by numbers of citations. U.S. chemists also lead in the quality of their publications. The total citations of U.S. chemistry papers between January 1996 and November 2006 accounted for about 28 percent of the world total as compared to 29 percent for the combined contribution of Germany, England, France, Italy, Spain, and the Netherlands. The United States also leads in the number of citations per paper. U.S. chemists are the most prolific authors in high-profile journals such as *Science Nature*, and the *Journal of the American Chemical Society*. U.S. chemists contributed to 50 percent of the 100 most frequently cited chemistry papers, while Western Europe contributed 41 percent. Fifty percent of the world's most frequently cited chemists are from the United States.

In a further effort to characterize the leading chemists in the world, the panel asked experts from the United States and abroad to identify the "best of the best" whom they would invite to an international conference in their subfield. The national makeup of these "virtual congresses" provides another indicator of U.S. leadership in chemistry by the strong predominance of U.S. speakers (50-70 percent) selected for virtual world congresses. (*Caveat:* When the organizer of the virtual congress was a U.S. chemist, about 15 percent more of the speakers were from the United States than when the organizer was not from the United States.)

Analysis of publications and virtual congresses showed that U.S. chemistry is particularly strong in emerging cross-disciplinary areas such as nanochemistry, biological chemistry, and materials chemistry.

A Combination of Factors Is Responsible for U.S. Research Leadership in Chemistry

Many factors influence U.S. research leadership in chemistry. One of the main factors is the national instinct to respond to external challenges,

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to encourage innovation, and to compete for leadership. The wide range of funding sources for support of academic chemistry research (including industry, multiple federal agencies, state initiatives, universities, and private foundations) facilitates innovative research. Key characteristics of the U.S. scientific culture that underlie current and future leadership in chemistry research include cross-sector collaborations and international partnerships, strong professional societies, early full independence of investigators, and mobility across academic institutions. Major centers and facilities provide key infrastructure and capabilities for conducting research and have provided the foundation for U.S. leadership. There is increasingly strong competition for international scientists and engineers. The United States has maintained a steady supply of Ph.D. chemistry graduates by increasingly relying on foreign-born students. Over time the number of U.S. citizens pursuing chemistry Ph.D. degrees has declined. Research funding for chemistry has been steady, but an increasing percentage of support for U.S. chemistry research is coming from a single source, the National Institutes of Health.

Chemistry Research in the United States Is Projected to Remain Stronger in the Next Decade than in Any Other Single Country, but Competition Is Increasing

In the near future, U.S. chemistry will be the "leader" or "among world leaders" in all areas, but not in all subareas. Because of the advance of chemistry in other nations, competition is increasing; and the lead of U.S. chemistry will shrink. There will be increasing competition from our traditional European competitors, the expanding European Union, Japan, and other Asian countries, particularly China and India. U.S. leadership in chemistry publications will continue to diminish. As U.S. publication rates remain steady, the number and quality of papers from other countries are increasing.

U.S. Chemistry Will Be Particularly Strong in Emerging Areas

Areas such as nanoscience, biological chemistry, and materials chemistry continue to attract new investigators and funding initiatives. Even in these areas, the U.S. leadership position may erode due to growing competition. At the same time, the growth in applications-oriented research has been accompanied by a parallel decrease in funding for basic research in some fundamental core areas of physical, inorganic, and organic chemistry.

U.S. Chemistry Leadership Will Diminish in Core Areas

Core research areas, which underlie advances in emerging areas of science, are likely to continue to struggle for research support. Japan and Eu-

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rope maintain more balanced support between core and emerging areas of chemistry. In some core subareas, such as main group chemistry and nuclear and radiochemistry, the U.S. position has already noticeably diminished based on publication and citation rates, and on virtual congress results.

The Sustainability of the Supply of U.S. Chemists May Be in Jeopardy

It is likely that the number of U.S. citizens receiving chemistry Ph.D.s will continue to decrease. At the same time, U.S. chemistry may find it increasingly difficult to attract and retain outstanding international graduate students and postdoctoral research associates as chemistry and opportunities in other nations improve. The U.S. will find it difficult (but not impossible) to increase the number of B.S. chemists and to improve the quality of K-12 math and science education to preserve the medium and long-term vibrancy of U.S. chemistry.

U.S. Funding of Chemistry Research and Infrastructure Will Remain Under Stress

U.S. funding of chemistry is projected to continue to barely keep up with inflation and to be concentrated in emerging and interdisciplinary areas. Core research areas of chemistry, which underlie advances in the emerging areas of science, will in all likelihood not be as well funded. Support available for the installation and operation of a diverse range of facilities to support leading-edge research in chemistry will be equally stretched thin.

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Why Benchmark the Research Competitiveness of U.S. Chemistry Research Now?

The National Academies is periodically asked to assess the effectiveness of research investments in addressing national concerns. Research investments in turn affect the quality of research done. In 2000 the National Academies explored a new way of evaluating research leadership status through an international benchmarking exercise[1] which compares the quality and impact of research in one country (or region) with world standards of excellence.

As Maxine Singer pointed out in the preface to that benchmarking exercise, "The American people, through their elected representatives, support the nation's research enterprise in the expectation of substantial returns on their investment: a higher standard of living, a healthier society, an environmentally sustainable economy, and a strong national security. Knowing the power of research in addressing national objectives, the nation has committed itself to a broad set of investments to uphold its research capability."

The pilot study of materials science, immunology, and mathematics was deemed successful in providing useful information to help inform science policy decisions in a rapid and low-cost way.

THE *RISING ABOVE THE GATHERING STORM* REPORT

More recently, the American people, Congress, and the President have had growing concerns about the competitiveness of the United States and

[1]National Research Council, 2000, *Experiments in International Benchmarking of U.S. Research Fields*, National Academy Press, Washington, D.C.

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its ability to lead the world in innovation and job creation. As a result of concerns that a weakening of science and technology in the United States would inevitably degrade its social and economic conditions and erode the ability of its citizens to compete for high-quality jobs, Senators Lamar Alexander and Pete Domenici asked the National Academies to select a committee of experts from the scientific and technical community to assess the current situation, identify urgent challenges, and recommend specific steps to ensure that the United States maintains its leadership in science and engineering to compete successfully.

The resulting report,[2] *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, evaluated the present status of U.S. competitiveness and made specific recommendations for improvements. A very short summary of the conclusions from the executive summary of that report is given in Box 1-1. In the first chapter of that report, some alarming competitiveness indicators are described. Several of relevance to chemistry are given here in Box 1-2.

TIMELINESS OF BENCHMARKING CHEMISTRY

Building on the results of these two studies, in 2006 the National Academies embarked on an effort to benchmark the research competitiveness of the United States in chemistry. In addition to concerns about the overall competitiveness of the United States, there are compelling reasons to assess the standing of U.S. chemistry now. The field of chemistry is facing issues of identity and purpose at a time when it is expanding beyond its traditional core to include areas related to biology, materials science, and nanotechnology. Concerns about the pipeline of students, about the nature of future employment opportunities, and about the fundamental health of the discipline and industry are regular topics of discussion at meetings of the American Chemical Society (ACS) and the Council for Chemical Research (CCR) and have been the topic of such exercises as Chemical Vision 2020 and Chemical Enterprise 2015.[3] Chemistry is facing a crucial time of change and is working to position itself to meet the needs of the future.

[2]National Research Council, 2007, *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, The National Academies Press, Washington, D.C.

[3]For more information about the CCR Chemical Vision 2020 technology road maps, see *http://www.chemicalvision2020.org/techroadmaps.html*. For the ACS Chemical Enterprise 2015 results, see *http://chemistry.org/chemistryenterprise2015.html*.

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BOX 1-1
Conclusions from the
***Rising Above the Gathering Storm* Report**

"The [Committee on Prospering in the Global Economy of the 21st Century] believes that its recommendations and the actions proposed to implement them merit serious consideration if we are to ensure that our nation continues to enjoy the jobs, security, and high standard of living that this and previous generations worked so hard to create. Although the committee was asked only to recommend actions that can be taken by the federal government, it is clear that related actions at the state and local levels are equally important for U.S. prosperity, as are actions taken by each American family. The United States faces an enormous challenge because of the disparity it faces in labor costs. Science and technology provide the opportunity to overcome that disparity by creating scientists and engineers with the ability to create entire new industries—much as has been done in the past.

"It is easy to be complacent about U.S. competitiveness and preeminence in science and technology. We have led the world for decades, and we continue to do so in many research fields today. But the world is changing rapidly, and our advantages are no longer unique. Some will argue that this is a problem for market forces to resolve—but that is exactly the concern. Market forces are *already at work* moving jobs to countries with less costly, often better educated, highly motivated workforces and friendlier tax policies.

"Without a renewed effort to bolster the foundations of our competitiveness, we can expect to lose our privileged position. For the first time in generations, the nation's children could face poorer prospects than their parents and grandparents did. We owe our current prosperity, security, and good health to the investments of past generations, and we are obliged to renew those commitments in education, research, and innovation policies to ensure that the American people continue to benefit from the remarkable opportunities provided by the rapid development of the global economy and its not inconsiderable underpinning in science and technology."

SOURCE: National Research Council, 2007, *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, The National Academies Press, Washington, D.C.

PANEL CHARGE AND RATIONALE

Before addressing questions of how chemistry must shift to meet future needs, it is imperative to understand its current health and international standing. At the request of the Department of Energy Basic Energy Sciences Chemical Sciences, Geosciences, and Biosciences Division, and the National Science Foundation Chemistry Division, the National Academies' Board on Chemical Sciences and Technology performed an international benchmark-

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BOX 1-2
Some Competitiveness Indicators of Relevance to the Chemical Sciences as Noted in the Executive Summary of *Rising Above the Gathering Storm*

U.S. Economy

- The United States is today a net importer of *high-technology* products. Its trade balance in high-technology manufactured goods shifted from *plus* $54 billion in 1990 to *negative* $50 billion in 2001.
- Some economists estimate that about half of U.S. economic growth since World War II has been the result of technological innovation.

Comparative Economics

- Chemical companies closed 70 facilities in the United States in 2004 and tagged 40 more for shutdown. Of 120 chemical plants being built around the world with price tags of $1 billion or more, one is in the United States and 50 are in China. No new refineries have been built in the United States since 1976.

K-12 Education

- In 1995 (the most recent data available), U.S. 12th graders performed below the international average for 21 countries on a test of general knowledge in mathematics and science.
- According to a recent survey, 86 percent of U.S. voters believe that the United States must increase the number of workers with a background in science and mathematics or America's ability to compete in the global economy will be diminished.

Higher Education

- In South Korea, 38 percent of all undergraduates receive their degrees in natural science or engineering. In France, the figure is 47 percent, in China, 50 percent, and in Singapore, 67 percent. In the United States, the corresponding figure is 15 percent.
- Some 34 percent of doctoral degrees in natural sciences (including the physical, biological, earth, ocean, and atmospheric sciences) and 56 percent of engineering Ph.D.s in the United States are awarded to foreign-born students.
- In the U.S. science and technology workforce in 2000, 38 percent of Ph.D.s were foreign-born.

Research

- In 2001 (the most recent year for which data are available), U.S. industry spent more on tort litigation than on research and development.
- Federal funding of research in the physical sciences, as a percentage of Gross Domestic Product, was 45 percent less in FY 2004 than in FY 1976.

SOURCE: National Research Council, 2007, *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, National Academies Press, Washington, D.C.

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ing exercise to determine the standing of the U.S. research enterprise in the field of chemistry relative to its international peers.

The field of chemistry was benchmarked by an ad hoc panel consisting of 13 members, 12 from the United States and one from Switzerland, with expertise across the 11 selected areas covered in the report (to be discussed in Chapter 2), which are analytical, atmospheric, biological, chemical education, inorganic, macromolecules, materials and nanomaterials and nanoscience, nuclear/radiochemistry, organic, physical, and theory/computation. The panel was charged with addressing three specific questions:

- What is the current position of U.S. chemistry research relative to that of other regions or countries?
- What key factors influence U.S. performance in chemistry?
- On the basis of current trends in the United States and abroad, what will be the relative U.S. position in the near term and in the longer term?

Following a process similar to that established in *Experiments in International Benchmarking of U.S. Research Fields*,[4] the panel was instructed to perform their charge in a short time frame and with a limited budget. The group met one time in person, and otherwise met via teleconference. Thus, in order to adequately respond to their charge, the panel had to limit the scope of the benchmarking exercise to assessing the state of basic (fundamental) chemistry research as determined by the open literature, the opinions of their peers in the United States and abroad, and other sources of easily accessible information. This benchmarking exercise was conducted based on the premise that evaluating this type of more "academic" research information would give a good estimate of the quality and quantity of fundamental research being conducted, which could in turn be used as an indicator of competitiveness of the larger chemical enterprise. However, this exercise in no way presents a complete picture of the level of research activity of the enterprise—particularly the industrial component.

The quantitative and qualitative measures employed to compare U.S. chemistry with that in other nations included analysis of journal publications (numbers of papers, citations of papers, most cited papers, most cited authors, most accessed papers), utilizing such sources as Thompson ISI Essential Science Indicators and data provided by the American Chemical Society Publications Division. In addition, the panel asked leading experts from the United States and abroad to identify the "best of the best" whom they would invite to an international conference in their subfield. The

[4]Committee on Science, Engineering, and Public Policy, 2000, *Experiments in International Benchmarking of U.S. Research Fields*, National Academy Press, Washington, D.C.

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national makeup of these "virtual world congresses" provided qualitative information on leadership in chemistry. International prizes and congresses were also considered. The panel steered clear of distinguishing between academic, industrial, and governmental laboratory research performers, all of whom were considered in the exercise.

Finally, the panel examined trends in the numbers of degrees, employment, and research funding of U.S. chemistry, relying heavily upon the NSF S&E Indicators 2006 and earlier years. The resulting report details the status of U.S. competitiveness of research in chemistry and its subareas. This benchmarking exercise attempts to determine the current status of the discipline and to extrapolate the future status based on current trends. The report does not make judgments about the relative importance of leadership in each area or make recommendations on actions to be taken to ensure such leadership in the future.

The outline of this report is as follows: Chapter 2 of this report will provide background on the key characteristics of chemistry. Chapter 3 responds to the first question of the panel charge, and details the panel's assessment of the current standing of the United States in the 11 areas of chemistry. Chapter 4 addresses the second question of the charge and identifies the key determinants of leadership in the field. Chapter 5 addresses the third part of the charge, assimilating past leadership determinants and current benchmarking results to predict U.S. leadership. Will the United States gain, maintain, or lose its competitive position? The panel's predictions for each of the chemistry areas are also assessed.

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2

Key Characteristics of U.S. Chemistry Research

Chemists view the world at the atomic and molecular levels. They relate the properties of all substances to the detailed chemical compositions and atomic arrangements of all the chemical components. Understanding how the properties of substances are related to their molecular structures helps chemists design new molecules and materials that have the desired properties, allows them to develop or invent *new* types of transformations for carrying out the syntheses of these substances, and assists in designing ways to manufacture and process the new substances and materials.

A 2003 National Research Council report, *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering* described some of the key structures and cultures of the disciplines and "the common chemical bond" that joins the two.[1] Chemistry was described as an unusual natural science that pursues both *discovery* and *creation*. Chemists seek to discover the components of the chemical universe—from molecules to organized chemical systems such as materials, living cells, and whole organisms—and to understand how these components interact and change over time. Synthetic chemists create new substances unknown in the natural world and develop novel transformations needed to make them. Chemical scientists produce tangible benefits to society when they design and engineer useful substances, such as new pharmaceuticals and polymeric materials.

[1]National Research Council, 2003, *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering*, The National Academies Press, Washington, D.C.

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WHAT IS CHEMISTRY RESEARCH?

Chemists are concerned with the physical properties of substances. Are they solids, liquids, or gases? How much energy do they contain? Chemists are also concerned with chemical properties. Can they be transformed to other substances on heating or irradiating? What are the detailed mechanisms of these transformations?

Chemical scientists also seek to understand the biological properties of both natural and man-made substances. They strive to understand the molecular basis of life processes. Furthermore, chemical science is integral to all of bioengineering and biotechnology. Biosystems, from molecular assemblies to cells to organisms, require insight from synthetic and physical chemistry as well as analysis of complex chemical networks if they are to be understood and exploited for the benefit of society.

The *Beyond the Molecular Frontier* report provided a list of "Grand Challenges for Chemists and Chemical Engineers" that highlights modern issues in the chemical sciences. (See Box 2-1.)

WHAT KEY FACTORS CHARACTERIZE CHEMISTRY RESEARCH?

Chemists have historically specialized in standard subdivisions: analytical, biochemical, inorganic, organic, physical, and theoretical. Increasingly, the boundaries between areas of chemistry and between chemistry and other disciplines are blurring. While some chemists focus on fundamental problems in core areas, an increasing number of chemists are using multidisciplinary approaches to solve problems at the interfaces with biology, physics, or materials science. For the purposes of this report, chemistry has been divided into 11 areas, most with multiple subareas, to assess the U.S. strength in modern chemistry. (See Box 2-2.) The report from a related benchmarking study of chemical engineering should be seen for more information on the U.S. standing in green chemistry/engineering, sustainability, and energy production.

Academic chemists have traditionally operated as single investigators with a team of graduate students and postdoctoral research associates, but increasingly academic chemists are joining larger multidisciplinary teams that bring together chemists and scientists from other scientific and engineering areas (see Figure 4-1). Partnerships between industrial, university, and government laboratories are becoming more common. International collaborations made possible by improved Internet communications also are becoming more common.

Research in chemistry is often capital intensive and involves increasingly sophisticated instruments and equipment for synthesis, processing, characterization, and analysis. Such equipment ranges from simple labora-

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BOX 2-1
Some Grand Challenges for Chemists and Chemical Engineers

- Learn how to synthesize and manufacture any new substance that can have scientific or practical interest, using compact synthetic schemes and processes with high selectivity for the desired product, and with low energy consumption and benign environmental effects in the process.
- Develop new materials and measurement devices that will protect citizens against terrorism, accident, crime, and disease, in part by detecting and identifying dangerous substances and organisms using methods with high sensitivity and selectivity.
- Understand and control how molecules react—over all time scales and the full range of molecular size.
- Learn how to design and produce new substances, materials, and molecular devices with properties that can be predicted, tailored, and tuned before production.
- Understand the chemistry of living systems in detail.
- Develop medicines and therapies that can cure currently untreatable diseases.
- Develop self-assembly as a useful approach to the synthesis and manufacturing of complex systems and materials.
- Understand the complex chemistry of the earth, including land, sea, atmosphere, and biosphere, so we can maintain its livability.
- Develop unlimited and inexpensive energy (with new ways of energy generation, storage, and transportation) to pave the way to a truly sustainable future.
- Design and develop self-optimizing chemical systems.
- Revolutionize the design of chemical processes to make them safe, compact, flexible, energy efficient, environmentally benign, and conducive to the rapid commercialization of new products.
- Communicate effectively to the general public the contributions that chemistry and chemical engineering make to society.
- Attract the best and the brightest young students into the chemical sciences, to help meet these challenges.

SOURCE: National Research Council, 2003, *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering*, The National Academies Press, Washington, D.C.

tory glassware and spectrophotometers, to sophisticated lasers, and from other instruments dedicated to a single investigator, to instruments such as nuclear magnetic resonance (NMR) spectrometers and mass spectrometers that serve a department or in some cases the entire country. Chemistry in the United States also benefits from a large base of research facilities, including synchrotron sources, nuclear reactors, and large-scale supercomputers. Computational research, involving supercomputers and computer

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BOX 2-2
Areas and Subareas of Chemistry Used in This Report

Analytical Chemistry
- Molecular and Surface Imaging
- Microfluidics and Miniaturization
- Sensors and Detectors
- Single-Cell Analysis
- Proteomics

Atmospheric Chemistry

Biological Chemistry
- Chemical and Structural Biology
- Biocatalysis
- Nucleic Acids and Functional Genomics
- Signaling Pathways
- In vivo Molecular Imaging

Chemical Education

Inorganic Chemistry
- Main Group Chemistry
- Organometallic Chemistry and Homogeneous Catalysis
- Bioinorganic Chemistry
- Solid State Chemistry

Macromolecular Chemistry
- Macromolecular Synthesis
- Physical Characterization of Macromolecular Systems
- Supramolecular Chemistry
- Rheology

networks, is gaining importance in solving a wide range of chemistry problems—from the subatomic to the macroscopic scale.

HOW IMPORTANT IS IT FOR THE UNITED STATES TO LEAD IN CHEMISTRY RESEARCH?

Chemistry is both a central science and an enabling science. It is often called on to provide scientific solutions for national problems. Chemistry plays a key role in conquering diseases, solving energy problems, ameliorating environmental problems, providing the discoveries that lead to new

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Materials Chemistry and Nanoscience
- Self-Assembly Science
- Nanocrystal and Cluster Science Nanomaterials: Energy and Applications
- Biomaterials/Bioinspired Materials Synthesis
- Bionano
- Tissue Engineering/Biocompatibility

Nuclear and Radiochemistry

Organic Chemistry
- Synthetic Organic Chemistry
- Physical Organic Chemistry
- Organocatalysis
- Natural Products Chemistry
- Medicinal Chemistry and Drug Discovery

Physical Chemistry
- Reaction Dynamics
- High-Resolution Spectroscopy
- Ultrafast Spectroscopy
- Biophysical Chemistry
- Heterogeneous Catalysis
- Single-Molecule Imaging and Electronics
- Surfaces and Interfaces Chemistry

Theory/Computation
- Electronic Structure/Basic Theory
- Molecular Dynamics Simulations
- Computer-Aided Chemical Discovery

industries, and developing new materials for national defense and new technologies for homeland security.

Medical research in particular is moving toward the molecular level, and rigorous chemistry is central to future progress in medicine. As outlined in the National Institutes of Health Roadmap for Medical Research,[2] current national priorities include new pathways to discovery in emerging and needed areas of research such as biological pathways (including metabolism) and networks; structural biology; molecular libraries and imaging;

[2]See *http://nihroadmap.nih.gov/*.

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nanotechnology; bioinformatics and computational biology—which cut across addressing all types of diseases and medical issues.

Chemistry is playing a central role in helping the United States attain energy independence. Almost all aspects of the national response to alternative energy issues involve chemistry—carbon dioxide sequestration, liquid fuels from coal, ethanol from corn and cellulose, the hydrogen economy, fuel cells, new battery concepts, and new concepts for solar energy. These involve energy storage and conversion into and out of chemical bonds. They also involve kinetics and multielectron catalysis. Solutions to energy problems will require a combination of basic research in chemistry with advanced chemical engineering and materials science. Chemists are now working to develop sustainable energy sources, including new photovoltaic devices and catalysts for the photo splitting of water into hydrogen and oxygen and synthetic systems that mimic natural photosynthesis. The greater utilization of nuclear energy will depend on chemists developing better ways for separating and storing nuclear waste. The new hydrogen economy will require chemists to develop better fuel cells and new ways of storing hydrogen. Chemists will be called on to play key roles in developing biofuels and will be needed to develop new materials from biomass to replace the use of petroleum-derived materials.[3]

While chemistry has inadvertently contributed to environmental problems, chemistry also is essential to improving our environment. Chemists have developed sensitive and specific analyses to monitor our environment, alternative environmentally benign pesticides and herbicides to aid agriculture, and new materials from renewable or recycled resources. Chemists aim to develop highly selective, energy-efficient, and environmentally benign new synthetic methods for the sustainable production of materials. New processes for synthesizing sustainable materials will have to be greener by design to reduce or eliminate the use and generation of hazardous substances. A success story involves the replacement of persistent chlorofluorocarbon refrigerants that led to the ozone hole. With replacements that are degraded in the lower atmosphere, the ozone hole is recovering.

The linkage between energy and climate will remain one of the most important challenges for the physical sciences for decades to come. It is certain the climate is warming, and chemistry will play a central role in understanding these changes and mitigating problems associated with global warming. Chemists are monitoring the increase in greenhouse gases such as carbon dioxide that lead to global warming and will be involved in numer-

[3]To see which Bush Administration initiatives in the past two years in research funding and public statement can be linked, go to *http://www.whitehouse.gov/news/releases/2006/01/20060131-6.html*.

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ous strategies to ameliorate global warming, including developing new energy sources and developing strategies for carbon dioxide sequestration.

WHAT ARE SOME CAVEATS?

There are well-known limitations associated with measures of scientific excellence, including publication and prize analysis. An additional problem arose for "virtual congresses," where the panel found small but significant differences depending on whether the organizer was from the United States or not.

There are also important factors that are advantageous for chemistry in the United States that must be taken into account when analyzing the state of the field of chemistry. English is the dominant language for chemistry research and publications, likely stemming from the historical U.S. dominance of the field of chemistry. This historical U.S. dominance has also been the major contributing factor for the literature dominance of ACS journals, which are highly regarded and enjoy great popularity as indicated by their associated impact factors. A strong case can be made that the dominance of the United States in the field of chemistry has been historically tied to the prominence of ACS journals, and the choice of English as the language of chemistry.

Because of the sheer size and strength of the U.S. chemistry research community, it cannot be compared meaningfully with those of other single countries. The only sensible method is to compare the United States with regional groups within Europe or Asia. To the extent possible, in this report, specific countries are mentioned in connection with particular areas of chemistry. While ample data were available on human resources and research funding for the United States, the panel had little comparable data for Europe and Asia.

With the enormous breadth of the chemical sciences, it was necessary to divide chemistry into 11 areas, each of which is also extremely broad. Undoubtedly, some areas have been left out. The U.S. standing in green chemistry/engineering, sustainability, and energy production was not addressed because the subjects are being covered extensively in the related benchmarking study of U.S. chemical engineering research.

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3

Current Research Leadership Position

To determine the overall position of U.S. research in chemistry relative to research performed in other regions or countries, the panel analyzed journals (paper authorship, most highly cited articles, most accessed articles, and hot papers), international congress speakers, and prizes. Most of these measures have previously been used to assess quality of science; however, in addition, the panel used virtual congress evaluations to determine the leadership groups within each subarea. The limitations of each individual measure were recognized, and therefore, the panel analyzed the collective results of all of the indicators to draw conclusions regarding relative research competitiveness.

APPROACH

In this part of the overall benchmarking study, the panel tried to collect objective information as much as possible, but it also recognized its responsibility for making collective subjective judgments when needed. In addition, certain boundaries were needed to keep the exercise timely and relevant to the broad chemical enterprise.

In this exercise the panel considered individual countries and geographic regions, which include the United States (including Puerto Rico and any U.S. territories), Canada, Western Europe (including Greece), Japan, Asia, and "Other."[1]

[1] "Asia 13" includes Bangladesh, China (including Hong Kong), India, Indonesia, Malaysia, Pakistan, the Philippines, Singapore, South Korea, Sri Lanka, Taiwan, Thailand, and Vietnam. "Europe 17" includes Austria, Belgium, Denmark, Finland, France, Germany, Greece, Iceland, Ireland, Italy, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, and the United Kingdom. When data were gathered from different sources, the regional grouping of nations was sometimes inconsistent, hence producing the differences in the nomenclature used for the country groups.

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The assessment begins with an overall view of leadership in chemistry at large, looking broadly at science and engineering (S&E) and chemistry research outputs. This largely includes an analysis of journal articles and citations, virtual congress results, and to a lesser extent, information on international congresses and prizes. Finally, the areas of chemistry are described and assessed.

JOURNAL ARTICLE CONTRIBUTIONS

Publication of research results is essential for scientific and technological progress and leadership. Thus, looking at quantity and quality of journal articles being published in the world is one important and largely objective measure of scientific research leadership. For this analysis the panel selected a list of leading journals, with high impact factors. The impact factor is a measure of the frequency with which the "average article" in a journal has been cited. The impact factor of a journal is calculated by dividing the number of current year citations to the source items published in that journal during the previous two years. Given the broad range of journals in which chemists publish, and in an effort to assess current trends in the directions of fundamental chemistry research, the panel selected the journals as follows:

- Journals with broad coverage of S&E disciplines, in which chemists publish (e.g., *Science*, *Nature*)
- Journals with broad coverage of chemistry (e.g., *Journal of the American Chemical Society*, *Angewandte Chemie*)
- Leading journals for each subarea of chemistry:
  - –Area-specific journals where chemistry researchers are the primary contributors (e.g., *Analytical Chemistry*, *Inorganic Chemistry*)
  - –Area(s)-specific journals where researchers from various sciences and/or engineering disciplines publish, along with researchers from chemistry (e.g., *Nature Materials*, *Physical Review Letters*)

The full list of all journals considered by the panel is given in Table C-1 in Appendix C.

The panel focused its analysis of journal publications data on the following metrics:

- Publication rates over roughly the past 15 years (1988 to present) in all of science and in chemistry.
- Percent contributions by U.S. researchers in all areas of science versus those from other countries or regions.

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- Percent contributions by U.S. chemists versus those of chemists from other regions.
- Percent of papers in the list of 100 most cited papers for the periods 1990-1994, 1995-1999, and 2000-2006.

To assess research leadership the panel concentrated on percent of hot papers, percent of highly cited papers, and the virtual congress results, which will be defined in more detail later in the report. For these criteria the following metric was used:

- Greater than 75 percent: the strong leader
- Greater than 50 percent: the leader
- Greater than 30 percent: among the leaders
- Less than 30 percent: lagging behind the leaders

Here, we first look at the numbers of journal articles being published in S&E overall, in chemistry, and finally in chemistry area-specific journals. It is important to note that the overall percentage of papers contributed by a particular country indicates only the quantity of work performed, rather than quality. That is why numerous other metrics were applied to the assessment to gauge the quality of the chemistry research produced by each country.

Decreasing U.S. Share of S&E Journal Articles

Examination of the number of articles published annually in the scientific literature on a regional basis shows that the profile of scientific activity worldwide has changed dramatically over the past 15 years (see Figure 3-1). The long-standing scientific dominance of the United States persists, but other areas of the world are closing the gap. In 1988 the United States was the largest contributor to S&E publications, even when compared to other regions. While the absolute number of U.S. S&E papers grew by 19 percent between 1988 and 2003, the output of articles from Western European nations combined increased by 67 percent and surged past the U.S. total. Dramatic growth was seen for papers from Korea, which grew 1,683 percent from 771 to 13,746; China, 630 percent from 4,001 to 29,186; and Taiwan, 556 percent from 1,414 to 9,270. The percentage of papers from Asia and the subcontinent as a whole, which include China and India, has increased by a factor of 2.5, from 4 percent to 10 percent of all articles. The percentage of all S&E articles from U.S. authors dropped from 38 to 30 percent between 1988 and 2003.

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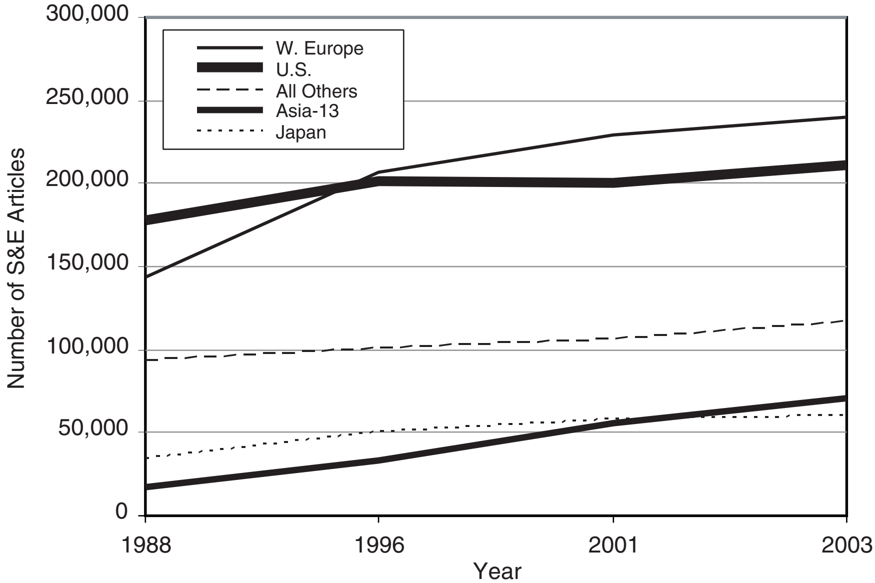

FIGURE 3-1 Numbers of all S&E articles for select countries and regions.
NOTE: Publication counts from set of journals classified and covered by Science Citation Index and Social Sciences Citation Index. Articles assigned to region/country/economy on the basis of institutional address(es) listed in article. Articles on fractional-count basis; i.e., for articles with collaborating institutions from multiple countries/economies, each country/economy receives fractional credit on the basis of proportion of its participating institutions.
SOURCE: Regional and country portfolio of S&E articles, 1988, 1996, 2001, and 2003. National Science Foundation, *2006 Science and Engineering Indicators*.

The Fastest-Growing Economies Have Increased Their Share of U.S. Patent Applications

While the number of U.S. patent applications from U.S. inventors more than doubled from 91,000 in 1990 to 189,000 in 2003, the percentage held steady at 55 percent.[2] In contrast, U.S. patent applications from the fastest-growing economies (China, Hong Kong, India, Ireland, Israel, Singapore, South Korea, and Taiwan) increased more than eightfold from 3,800 in 1990 to 30,800 in 2003; their share of U.S. patent applications more than tripled, from 2.3 to 9.0 percent.

[2]National Science Foundation, 2006, "U.S. Patent Applications, by Country/Economy of Origin of First-Named Inventor: 1990–2003 (Appendix Table 6-13)," *Science and Engineering Indicators 2006*.

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TABLE 3-1 Top 10 Chemistry Paper Producing Countries (for 10-Year Period, Jan. 1996 to Nov. 2006)

Rank	Country	Population (2006 est. in millions)	Chemistry Papers	Chemistry Papers/Million Inhabitants	Total Papers
1	United States	300	217,791	726	2,831,004
2	Japan	128	117,085	915	771,573
3	Peoples Republic of China	1,300	102,047	78	400,917
4	Germany	82	95,815	1168	723,435
5	France	61	64,121	1051	522,015
6	Russia	143	60,765	425	280,480
7	England	61	57,199	938	643,557
8	India	1,100	47,556	43	203,989
9	Spain	40	40,179	1004	254,808
10	Italy	58	39,141	675	358,452

SOURCE: Thomson ISI Essential Science Indicators and U.S. Census Bureau, International Database.

Decreasing U.S. Share of Chemistry Papers

The number of a nation's chemistry papers provides a quantitative measure of research activity in chemistry. According to Thomson ISI (which counts chemistry papers somewhat differently than the National Science Foundation (NSF)), U.S. chemists published more papers than those from any other country between 1996 and 2006 (see Table 3-1), accounting for about 18 percent of the total papers.[3] The U.S. total is nearly twice that of second-ranked Japan. However, in looking at the numbers of chemistry papers published per million inhabitants, Germany ranks first and the United States is sixth. In addition, compared to other regions (see Figure 3-2), the United States ranks second to Western Europe and just slightly ahead of Asia.

The trends in publication of chemistry papers show a leveling of U.S. activity in chemistry and growth in the rest of the world, except for the former Soviet republics (see Figure 3-3). Over the past decade the number of U.S. chemistry papers has remained relatively steady at about 15,000 annually. According to the NSF data shown, between 1988 and 2003 the percentage of articles contributed from both Western Europe and the United States dropped somewhat (from 22.9 to 19.1 percent for the United States), while the percentage from Asia (not Japan) more than tripled and now nearly matches the U.S. contribution.

[3]According to Tomson ISI Essential Science Indicators accessed on November 15, 2006, the total sum of papers from 89 major contributing countries listed was 1,223,166.

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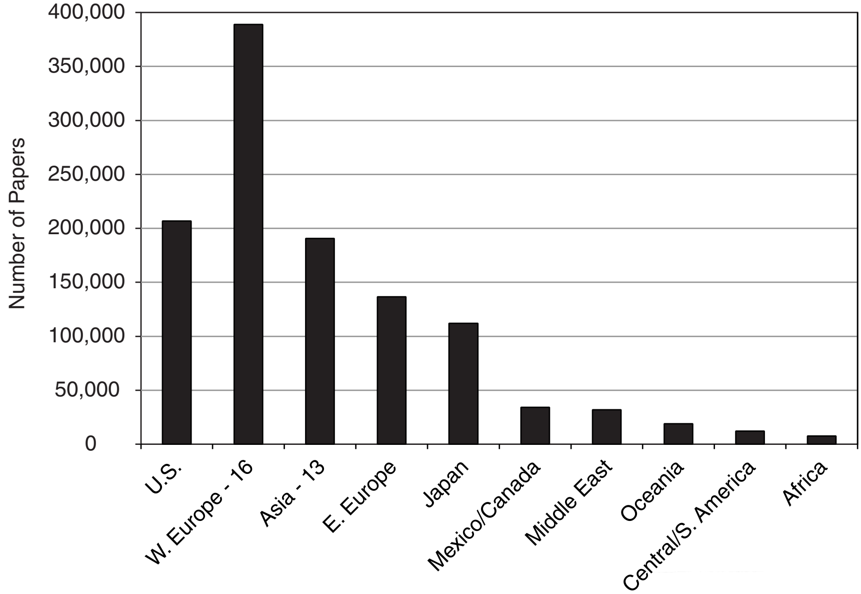

FIGURE 3-2 Comparison of select country and regional production of chemistry papers, 1996 to June 2006.
SOURCE: Thomson ISI Essential Science Indicators.

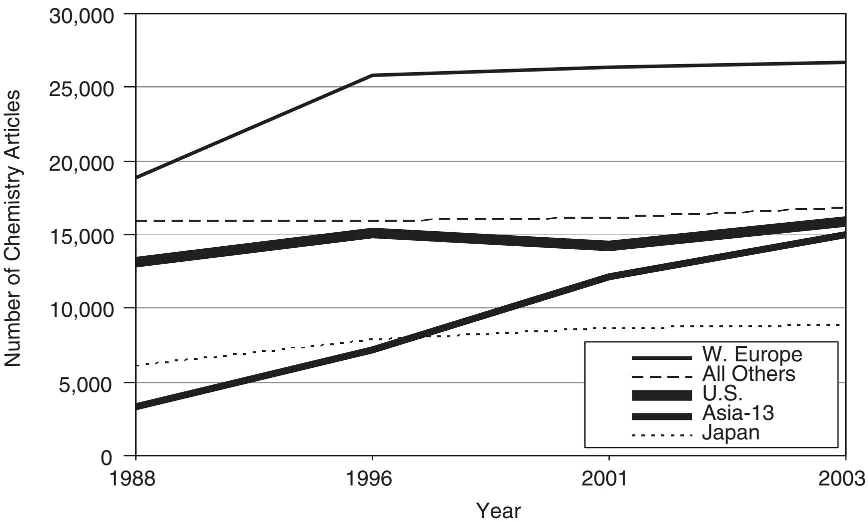

FIGURE 3-3 Numbers of chemistry articles published in the world for select countries and regions.
SOURCE: Regional and country portfolio of S&E articles, 1988, 1996, 2001, and 2003; National Science Foundation, *2006 Science and Engineering Indicators*.

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Figure 3-4 illustrates changes occurring in the contribution of U.S. and non-U.S. authors to American Chemical Society (ACS) journals. Since ACS journals are largely published in the United States by a U.S. organization, it is expected that U.S. authors would make the greatest contribution to these journals. However, the percentage of papers published by non-U.S. authors in American Chemical Society (ACS) journals has increased from 57 to 61 percent in the past six years shown. Contributions from Asia (largely due to China) doubled, from 6 to 12 percent. The increase in international papers in ACS journals reflects both the increasing popularity of the journals and the increasing ease of submitting papers electronically. It also indicates that the quality of non-U.S. papers is improving.

Figure 3-5 shows the declining percent contributions of U.S. authorship in ACS journals for specific areas of chemistry.

Chemistry Has a Small but Steady Share of U.S. S&E Article Output

Only 8 percent of U.S. S&E articles are in chemistry, compared to the world average of 12 percent (see Figure 3-6). While the United States contributes 30 percent of the S&E articles, it contributes only 19.1 percent of the chemistry articles. The U.S. position may be indicative of a more diverse research portfolio or an emphasis on biomedical-related fields (see Figure 3-5). This trend may also be related to an increasing number of

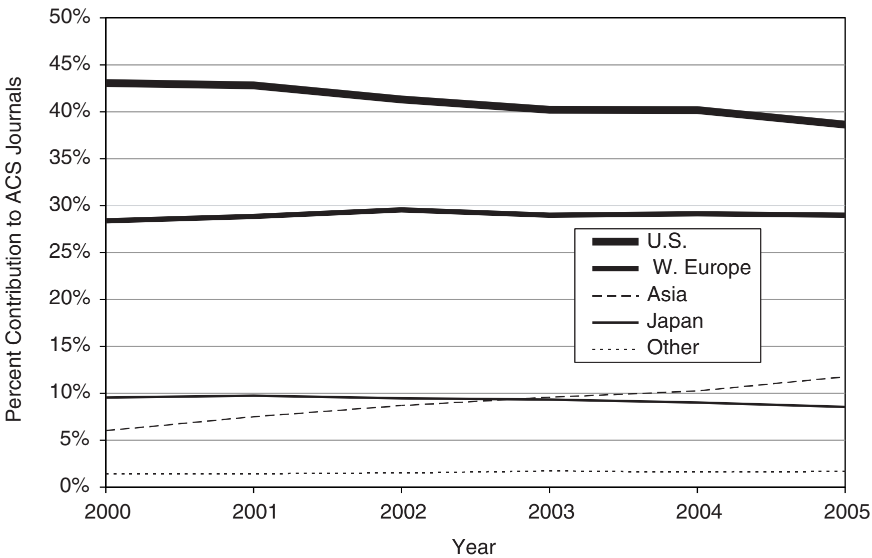

FIGURE 3-4 Percent contribution to all ACS journals from select regions.
SOURCE: American Chemical Society, Publications Division.

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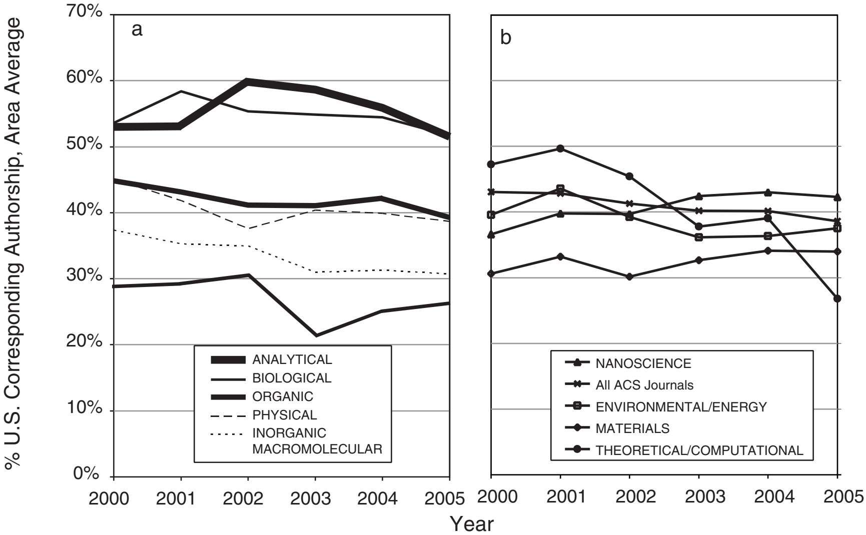

FIGURE 3-5 Percent contributions of U.S. authors to ACS journals by (a) traditional and (b) emerging areas of chemistry.
SOURCE: Analysis of data provided by ACS Publications Division.

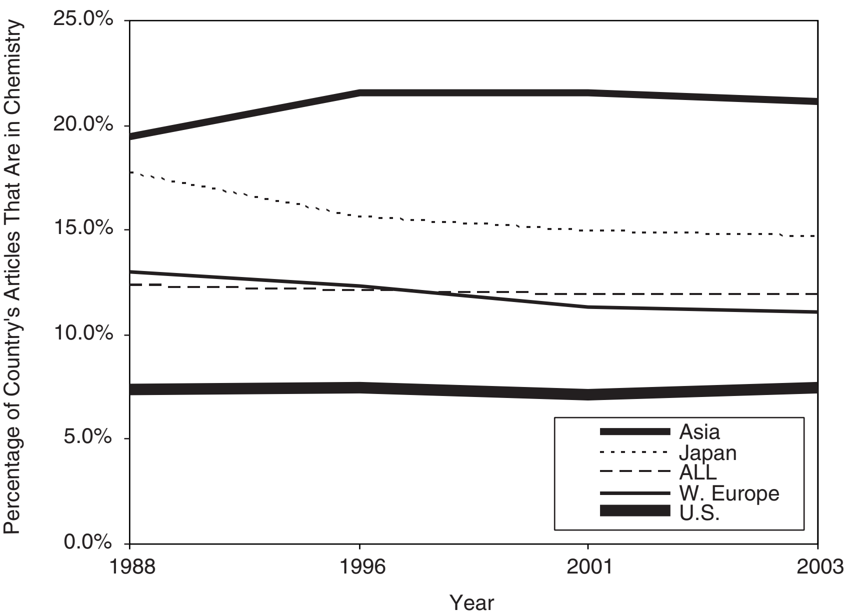

FIGURE 3-6 Percentage of a country's articles that are in chemistry.
SOURCE: Regional and country portfolio of S&E articles, 1988, 1996, 2001, and 2003; National Science Foundation, *2006 Science and Engineering Indicators*.

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publications in leading journals of other disciplines, due to the highly multidisciplinary nature of chemistry, especially in the United States.

Figures 3-7, 3-8, and 3-9 show the different research portfolios of the United States, China, and India for 1996 and 2003.

So far only data on the number of articles published in all of S&E and then in chemistry have been presented. The next section presents data that measure the impact and quality of publications. This information provides another measure of research leadership.

JOURNAL ARTICLE CITATIONS

This section looks at research quality through further analysis of article citations and papers deemed "hot" by Thomson ISI or that are most accessed through the ACS website.

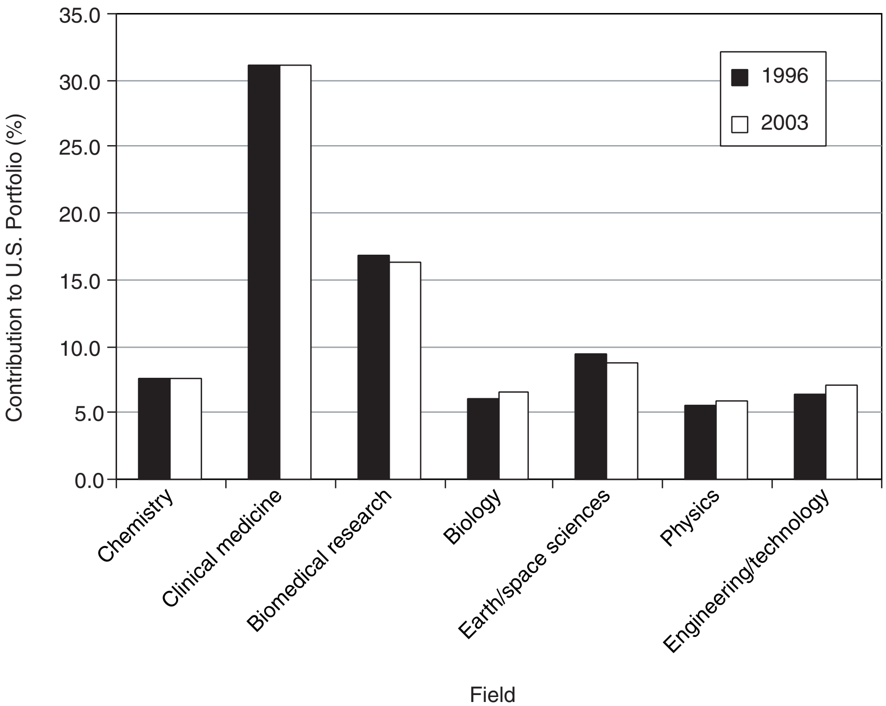

FIGURE 3-7 Research portfolio of the United States, 1996 and 2003.
SOURCE: National Science Foundation, *2006 Science and Engineering Indicators*.

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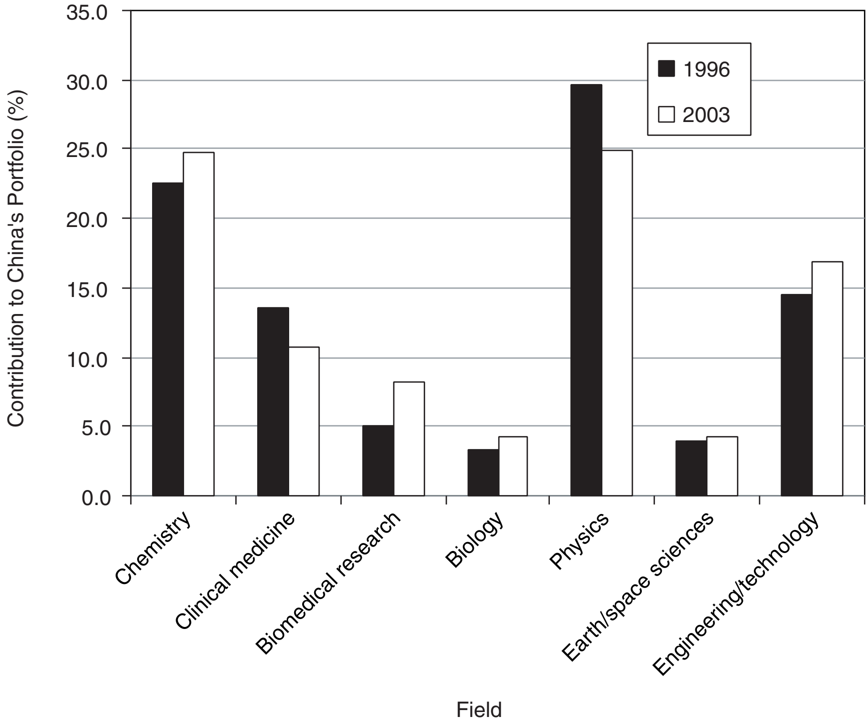

FIGURE 3-8 Research portfolio of China, 1996 and 2003.

Erosion of U.S. Lead in Journal Article Citations in Science and Engineering

As mentioned earlier, Western Europe surpassed the United States in total S&E publications in 1997. While the United States still leads Western Europe in number of citations, the gap is narrowing (see Figure 3-10). The erosion of U.S. leadership in citations is due both to the increased number of publications and to the increased number of citations per paper from Europe. These data provide evidence that both the quantity and the quality of papers from Western Europe are increasing.

U.S. Chemistry Leads in Total Citations and Citations per Paper

The total number of citations of chemistry articles provides a measure of the strength of a nation's contributions to chemistry, and the number of citations per paper gives information on the average impact of a nation's chemistry papers. The United States ranks first both in total citations and in

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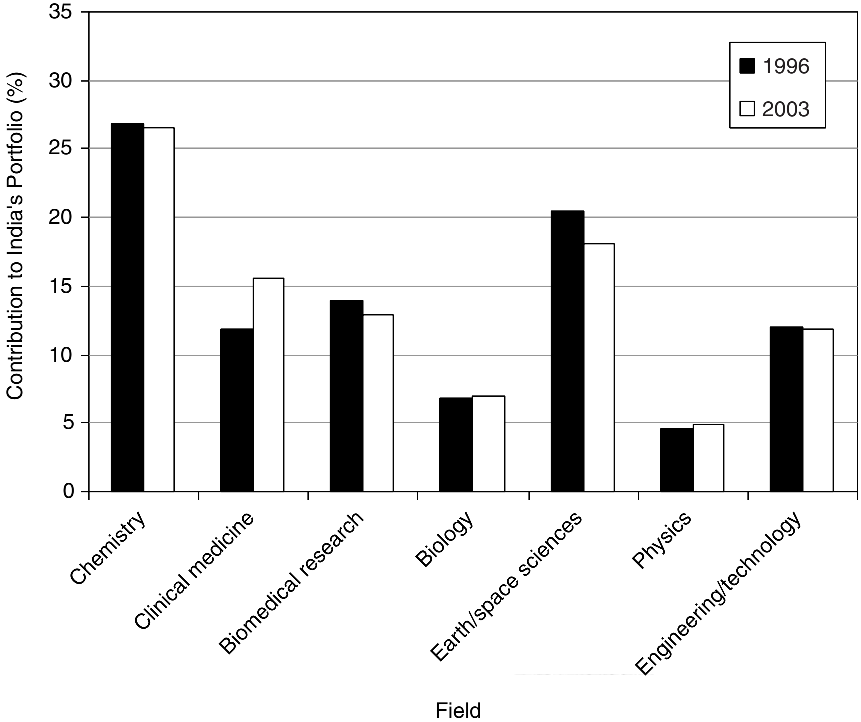

FIGURE 3-9 Research portfolio of India, 1996 and 2003.
SOURCE: National Science Foundation, *2006 Science and Engineering Indicators*.

citations per article in chemistry (see Table 3-2 and Figure 3-11). While U.S. authors published 18 percent of chemistry articles, their papers received 28 percent of the total world citations over the past 10 years.[4] Thus, although the United States lags behind Western Europe in terms of number of chemistry articles (Figure 3-3), the average impact of a U.S.-authored article, measured by citations, is substantially greater than for those from Western Europe and other regions.

Strong but Declining U.S. Contribution to Highly Cited Chemistry Articles

To assess the national origin of the highest-quality papers, the top 100 most highly cited papers in chemistry over the past 10 years were exam-

[4]According to Thomson ISI Essential Science Indicators (accessed November 15, 2006), the total sum of papers from the 89 major contributing countries listed was 10,654,721.

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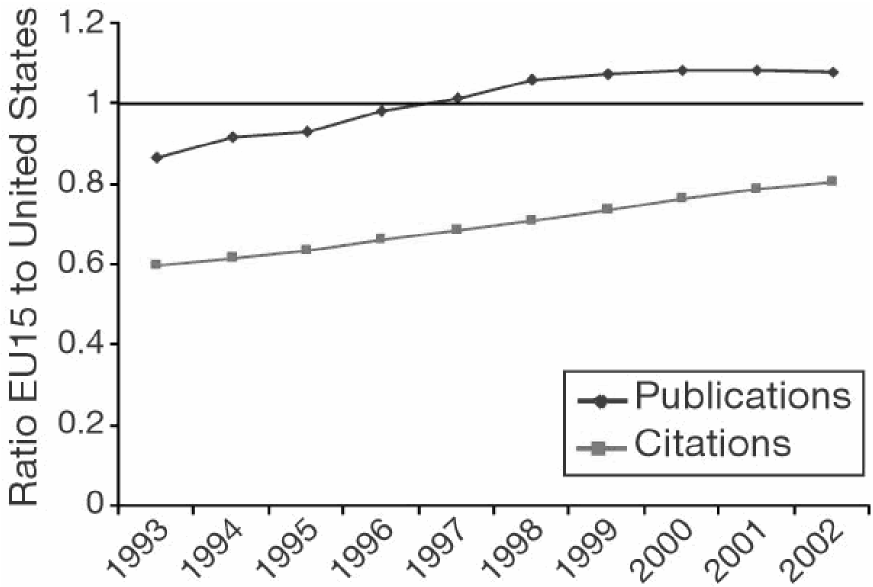

FIGURE 3-10 Ratio of publications and citations of the 15 European Union countries in the comparator group (EU15) to the United States on ISI databases 1993-2002.
NOTE: The EU15 total contains some duplication because of papers jointly authored between countries in the EU group. Counts for papers and citations are totals for country (or group) for the stated year.
SOURCE: D.A. King, "The scientific impact of nations," *Nature*, 430:311-316 (2004). Adapted by permission from Macmillan Publishers Ltd.

ined (see Figure 3-12). The leadership of the United States is shown by authorship of 50 percent of the papers. The strongest competition comes from Western Europe (consisting mostly of contributions from Germany, England, France, Spain, and Italy). The percentage of most highly cited papers shown here for the United States is two to three times greater than the percentage of U.S.-authored chemistry papers.

However, the U.S. share of highly cited papers shown in Figure 3-12 does not indicate whether the U.S. contribution is changing. To assess recent trends, the panel looked at the most frequently cited articles in a select group of chemistry journals. As shown in Figure 3-13, there was a slight decline in U.S. authorship from 53.5 to 47.2 percent from 1990-1994 to 2000-2006 and a nearly fourfold increase in Asian authorship from 1.5 to 5.6 percent (Asia includes India and China but not Japan).

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TABLE 3-2 November 2006 Ranking of Countries by Citations of Chemistry Articles and Citations per Paper (10-Year Period, 1996-2006)

Rank	Country	Citations (Chemistry)	Rank	Country	Citations Per Paper (Chemistry)
1	United States	3,028,796	1	United States	13.91
2	Japan	993,383	2	Switzerland	13.48
3	Germany	970,492	3	Netherlands	13.43
4	England	634,122	4	Denmark	12.76
5	France	606,563	5	Sweden	11.58
6	Peoples R China	402,036	6	Israel	11.48
7	Italy	366,694	7	Canada	10.83
8	Spain	350,279	8	Germany	10.13
9	Canada	322,083	9	Belgium	9.67
10	Netherlands	251,545	10	Australia	9.50

NOTE: Countries with less than 2,000 papers excluded.
SOURCE: Thomson Essential Science Indicators.

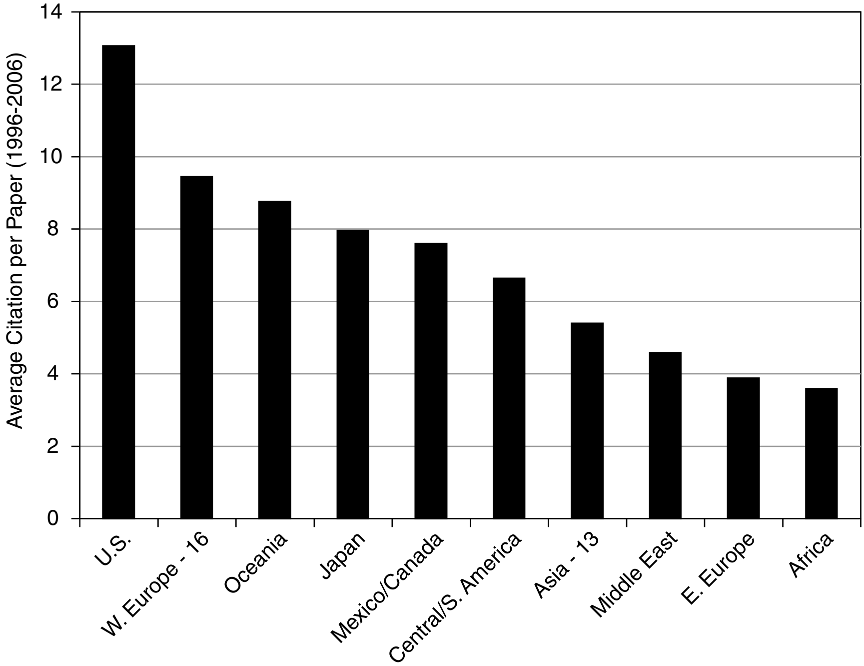

FIGURE 3-11 Highly cited countries and regions in chemistry (citations/article), 1996 through June 2006.
NOTE: ISI provides citation rankings for what are defined as chemistry-related journals based on past 10 years, plus partial-year counts for the current year. Data shown were collected in June 2006.
NOTE: E. Europe = Russia, Eastern Europe, former Soviet Bloc.
SOURCE: Thomson ISI Essential Science Indicators.

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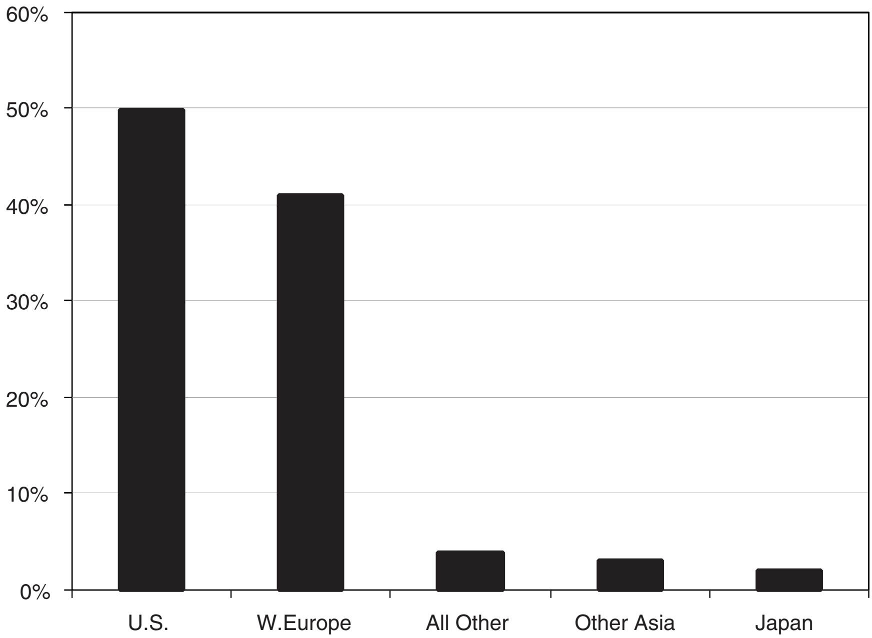

FIGURE 3-12 Percent contribution to top 100 most cited papers in chemistry for 1996-2006.
SOURCE: Thomson ISI Essential Science Indicators, accessed June 22, 2006.

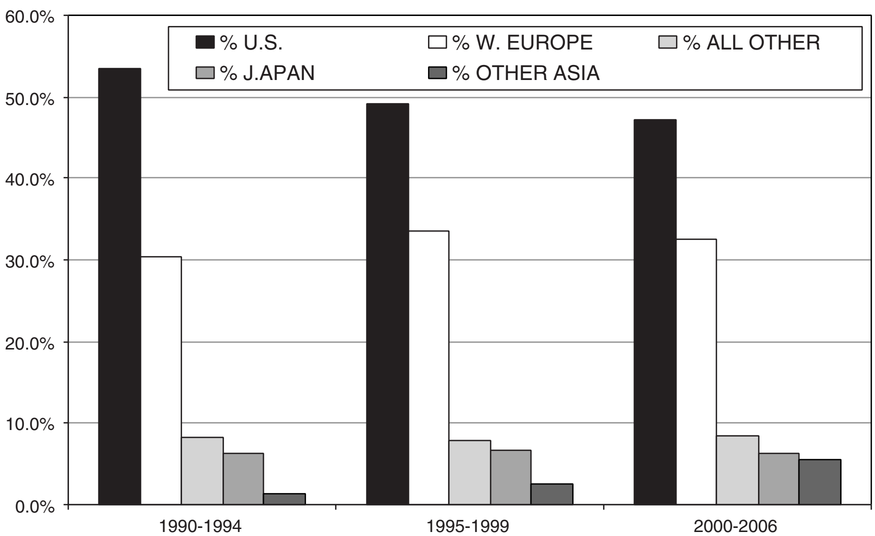

FIGURE 3-13 Regional/country breakout of most highly cited chemistry articles of all journals considered. (See also Appendix C, Table C-2.)

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U.S. contributions to the most cited articles in specific areas of chemistry are shown in Table 3-3. These results are discussed in more detail in the area assessments later in this chapter; however, it should be noted here that the trends in U.S. contributions vary significantly across the areas. While most areas show steady or declining U.S. contributions, analytical chemistry shows strong gains.

Strong and Steady U.S. Share of Highly Cited Chemists

Examination of the national origin of the most highly cited chemists provides another indication of a nation's strength in chemistry. About 50 percent of the most highly cited chemists are from the United States (Figure 3-14). This is a much larger percentage than the 19 percent U.S. contribution to all chemistry articles and the 28 percent U.S. contribution to all chemistry citations over the past 10 years.

Strong U.S. Contribution to Chemistry "Hot" Papers

The number of so-called hot papers provides another indicator of research quality. According to Thomson ISI, most papers reach their citation peak two to four years after publication, but some papers are recognized as hot and receive significant numbers of citations soon after publication. Often these papers are the key papers in their fields. Figure 3-15 shows country or regional contributions to the top 100 hot papers in chemistry

TABLE 3-3 Percent U.S. Authorship of Most Frequently Cited Articles in Journal Articles Compiled by Area of Chemistry

	1990-1994	1995-1999	2000-2006
U.S. %, Most Highly Cited by Area	U.S. %	U.S. %	U.S%
Multidisciplinary science	74.0	72.0	72.0
Multidisciplinary chemistry	48.0	27.6	37.2
Analytical chemistry	37.5	48.8	49.3
Biological chemistry	55.9	57.4	54.4
Chemical education		74.0	68.0
Environmental	49.0	36.7	30.0
Inorganic	51.0	38.5	40.5
Macromolecules	46.3	34.0	34.7
Materials science	33.0	44.5	41.2
Organic chemistry	59.5	58.8	47.0
Physical an computational	51.5	47.3	49.8
ALL	53.5	49.1	47.2

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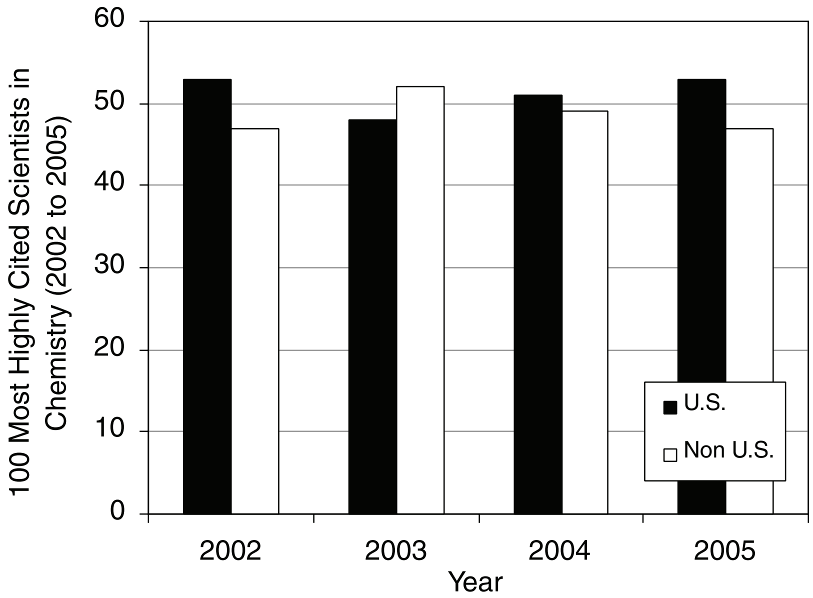

FIGURE 3-14 One hundred most highly cited scientists in chemistry.
SOURCE. Thomson ISI.

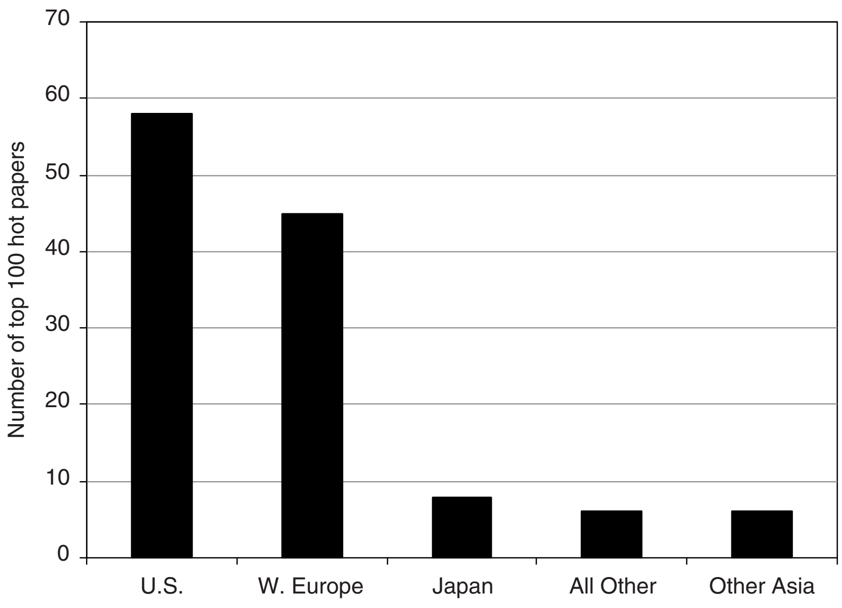

FIGURE 3-15 Top 100 hot papers in chemistry, 2004-2006.
SOURCE: Thomson ISI Essential Science Indicators.

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for 2004-2006. Once again, the United States shows strong leadership, with Western Europe following closely behind.

The largest number of hot papers in chemistry are in the areas of materials/nanoscience, organic chemistry, and inorganic chemistry (see Figure 3-16).

Although the U.S. contribution to hot papers is dominant, it varies significantly across the areas of chemistry (Figure 3-17). In the three areas of chemistry that dominate the hot papers, the United States contributed the most in materials/nanoscience, whereas Western Europe contributed the most in organic and inorganic chemistry.

Recently, the ACS has begun to highlight the top 20 "most accessed" articles in its journals. This provides another indication of where the most visible and highest-quality chemistry is being performed. As shown in Figure 3-18, U.S. chemists contribute the majority of the top 20 "most accessed" articles in ACS journals; however, four journals (*Biomacromolecules*, *Chem. Mater.*, *J. Med. Chem.*, and *Macromolecules*) had a less than 50 percent U.S. authorship of the most accessed articles. This analysis was performed for these ACS journals due to their quality and easily available data.

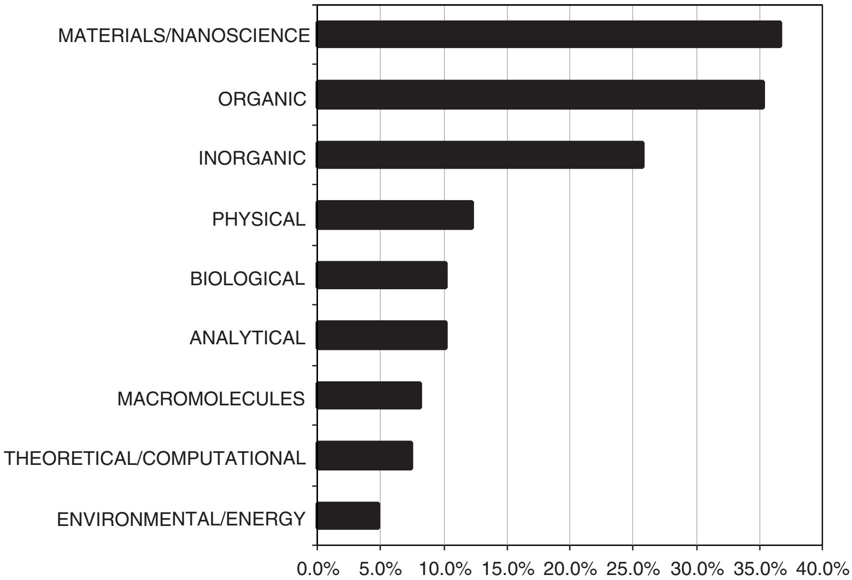

FIGURE 3-16 Distribution of top 100 hot papers among areas of chemistry, 2004-2006.
NOTE: Percentages do not total 100 because some papers were assigned to multiple areas.
SOURCE: Thomson ISI Essential Science Indicators.

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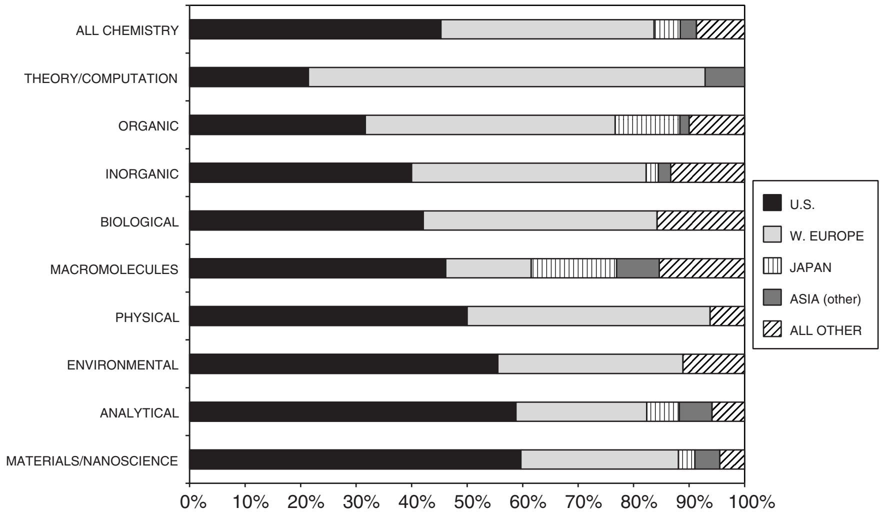

FIGURE 3-17 Country/region distribution of hot papers for the areas of chemistry. (List of hot papers by subarea given in Appendix C, Table C-2.)
SOURCE: Thomson ISI Essential Science Indicators.

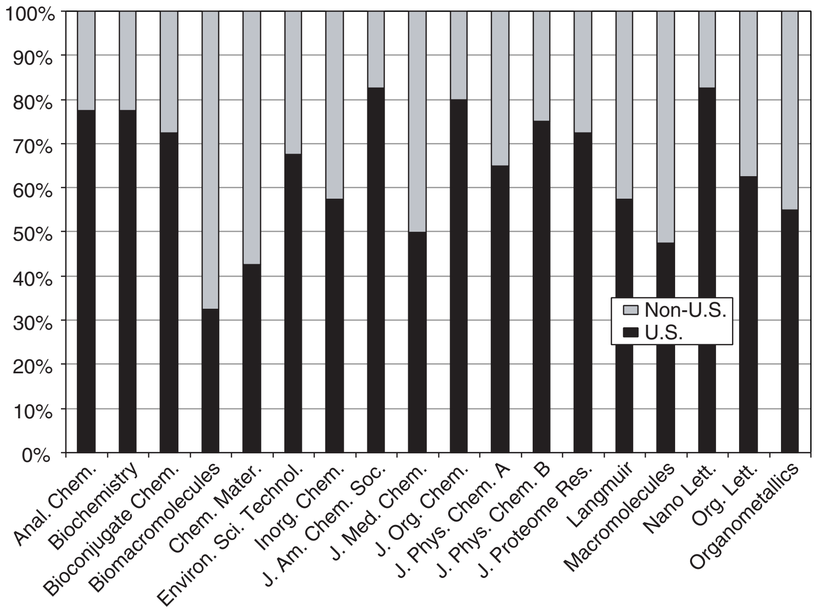

FIGURE 3-18 Percentage U.S. and non-U.S. most accessed ACS articles, 2004-2005.
SOURCE: ACS publications website (*pubs.acs.org*).

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OTHER MEASURES OF LEADERSHIP

In addition to the extensive look at journal articles published and cited, the panel assessed leadership in chemistry research through the virtual congress exercise, international congresses, and international prizes.

Strong U.S. Representation in Virtual World Congresses

In an effort to determine the leading chemists in the world, the panel called on an international group of chemists for their qualitative assessment of the subareas of chemistry. This exercise is referred to as the "virtual world congress."

To carry out the exercise, the field of chemistry was divided into 11 major areas. Each area was further subdivided into two to seven subareas. The panel then identified 8 to 10 respected leaders throughout the world in each subarea. These leaders were asked to imagine that they were to organize an international congress symposium on the subarea topic; then, regardless of travel costs, visa restrictions, or the opinions of their peers, they were asked who would be the 10 to 20 "best of the best" researchers in their subfields who must participate in the imaginary session.

The virtual congress data were used to characterize the relative position of the United States in each of the subfields. The panel considered the following criteria to assess research leadership as determined by the virtual world congresses:

- Greater than 75 percent: the strong leader
- Greater than 50 percent: the leader
- Greater than 30 percent: among the leaders
- Less than 30 percent: lagging behind the leaders

The strong predominance of U.S. speakers (50 to 70 percent) selected for the virtual world congresses shows strong U.S. leadership in chemistry (see Figure 3-19). Typically, when the organizer of the virtual world congress was a U.S. chemist, about 15 percent more of the speakers were from the United States than when the organizer was from elsewhere. These data will be discussed in more detail in the area assessment later in this chapter.

Large Percentage of U.S. Speakers at International Congresses

In another attempt to identify the world's leading chemists, the panel examined the lists of invited speakers at real (not imaginary) international chemistry meetings. The percentage of speakers from different countries

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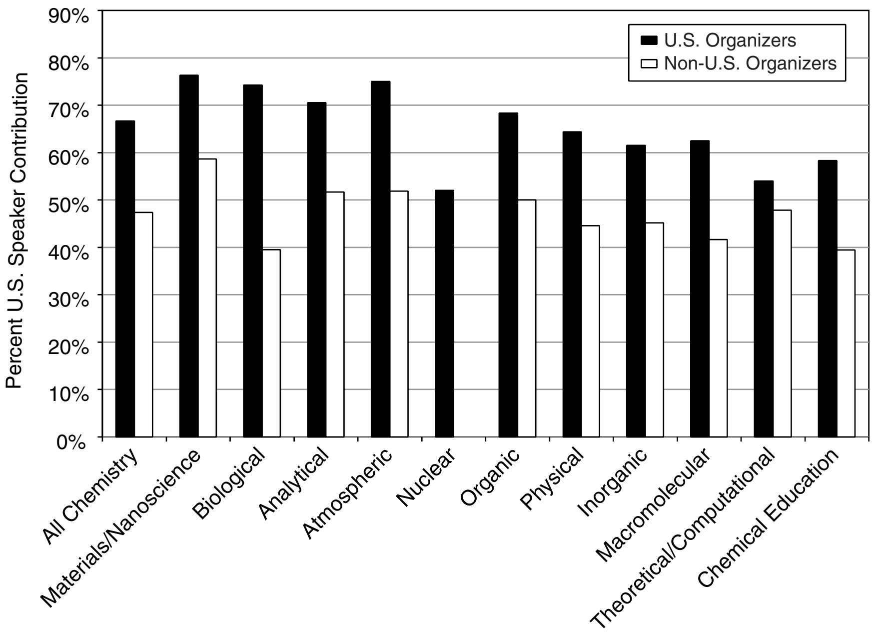

FIGURE 3-19 Percentage of U.S. speakers proposed by U.S. and non-U.S Virtual World Congress organizers.

was used to assess each nation's strength in chemistry research. As expected, the results were skewed toward a concentration of speakers from the same geographic area where the conference was held.

The panel looked at 46 international congresses that took place between 2004 and 2006. All 28 of the U.S. congresses and five of the non-U.S. congresses were Gordon Research Conferences (GRCs), which strive to "provide an international forum." The panel chose to concentrate on GRCs rather than other symposia because GRCs are small selective meetings that are highly regarded internationally for which speaker data were readily available. For the 28 U.S.-based GRCs, 70 percent of the speakers were from the United States (see Figure 3-20). For the 18 non-U.S. congresses, while only 30 percent of the speakers were from the United States, the U.S. contingent was larger than that of any other nation at these meetings.[5] It is evident from the speaker data that although they are international, GRCs are biased in favor of U.S. researchers, which the panel took into consideration.

[5]Appendix D lists the international congresses considered by the panel and the relative frequency of U.S. and non-U.S. chemists as invited plenary speakers.

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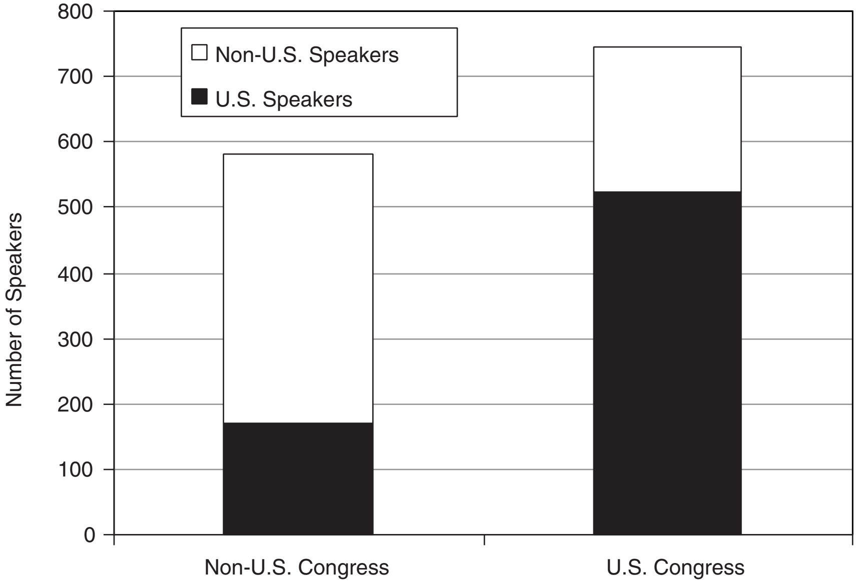

FIGURE 3-20 Number of invited speakers based on country affiliation and location of international congresses.

Gordon conference speakers are chosen from the leaders in a given subarea, and counting them should be an excellent benchmark of a country's status in the international arena. Sixty-eight percent of the 890 speakers at the 34 GRCs were from the United States. The composition of the five non-U.S. GRCs analyzed by the panel is shown in Figure 3-21.

Success of U.S. Chemists in Winning International Prizes

A nation's leadership in a scientific area is reflected in the number of its scientists who win major international prizes (see Tables 3-4 and 3-5). However, since prizes are sometimes awarded long after the recognized discovery, they are less informative about the current state of a nation's science. Between 2000 and 2006, 11 of 18 Nobel laureates in chemistry were U.S. scientists.

ASSESSMENT OF LEADERSHIP IN SPECIALIZED AREAS OF CHEMISTRY

This section looks more closely at the different areas and subareas in which chemists classify their research. These areas were chosen by the panel

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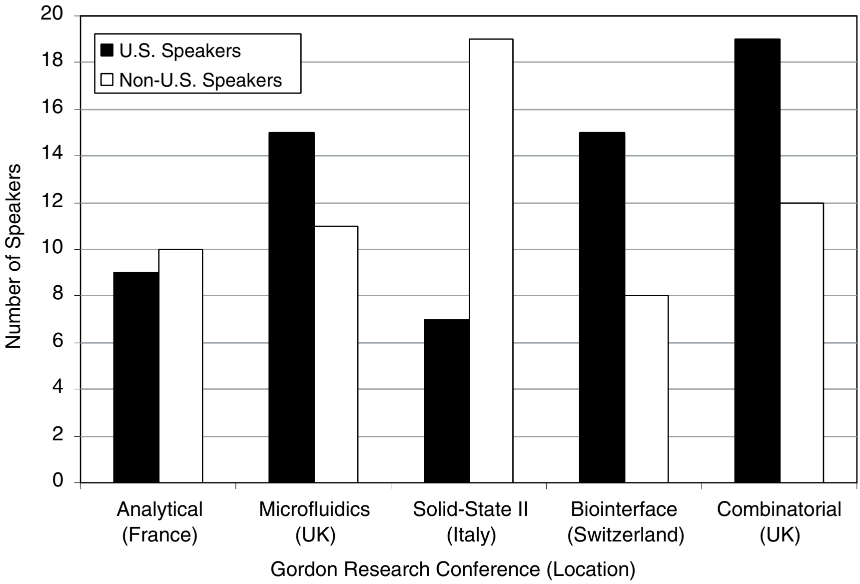

FIGURE 3-21 U.S. and non-U.S. participation as speakers at five chemistry GRCs held abroad.
SOURCE: National Research Council-generated tabulation of names listed on agendas on GRC website.

TABLE 3-4 2000-2006 Winners of Nobel Prize in Chemistry

Prize	Laureate	Citizenship	Research Done in
2000	Alan Heeger	United States	United States
	Alan MacDiarmid	United States and New Zealand	United States
	Hideki Shirakawa	Japan	Japan
2001	William Knowles	United States	United States
	Ryoji Noyori	Japan	Japan
	K. Barry Sharpless	United States	United States
2002	John Fenn	United States	United States
	Koichi Tanaka	Japan	Japan
	Kurt Wuthrich	Switzerland	Switzerland
2003	Peter Agre (M.D.)	United States	United States
	Roderick MacKinnon (M.D.)	United States	United States
2004	Irwin Rose	United States	United States
	Aaron Ciechanover	Israel	Israel
	Avram Hershko	Israel	Israel
2005	Richard Schrock	United States	United States
	Yves Chauvin	France	France
	Robert Grubbs	United States	United States
2006	Roger Kornberg	United States	United States

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TABLE 3-5 Other Major Science and Engineering Prizes Awarded to Chemists

Prize	Total Awardees	Total U.S. Awardees	Chemistry Awardees	U.S. Chemistry Awardees
Wolf (Chemistry)	6	4	4	4
Japan (2001-2006)	17	4	5	1
Kyoto	20	8	4	4

NOTES: The Wolf Prize is awarded by the Wolf Foundation in Israel (*http://www.wolffund.org.il/cat.asp?id=15&cat_title=CHEMISTRY*). Since 1978, five or six prizes have been awarded annually in the sciences. Prize fields are agriculture, chemistry, mathematics, medicine, and physics. The Japan Prize is awarded by the Science and Technology Foundation of Japan (*http://www.japanprize.jp/prize/prize_e1.htm*). This is awarded to people whose original and outstanding achievements in science and technology are recognized as having advanced the frontiers of knowledge and served the cause of peace and prosperity for mankind. Fields of study for the prize encompass all categories of science and technology. The Kyoto Prize is awarded by the Inamori Foundation, Japan (*http://www.kyotoprize.org/ or http://www.inamori-f.or.jp/index_e.html*), which is an international award to honor those who have contributed significantly to the scientific, cultural, and spiritual betterment of mankind. The prize is presented annually in each of the following three categories: advanced technology, basic sciences, and arts and philosophy. Laureates shall in principle be individuals (one person per category).

as representative of both the historic and future directions of the field of chemistry.[6]

The United States Is the Leader in Analytical Chemistry

Analytical chemistry is the science of measurement of chemical properties and chemical quantities. Analytical chemists determine the fundamentals of instrumental responses to chemical properties; invent instrumentation for molecular and atomic separation, characterization, and imaging; and develop a rigorous understanding of how to interpret experiments that characterize chemicals. Analytical chemistry interfaces strongly with other chemical, chemical engineering, biological, and physical sciences, through shared interests in the chemical structures and molecular compositions of complex systems, including nanodevices and living organisms. Analytical chemists' tools and interpretation provide diagnoses of diseases, assure the purity of pharmaceutical products, obtain forensic information, investigate global warming, and describe the human genome.

Five specialty areas were examined to assess the current status of the U.S. contribution to analytical chemistry. These five were selected because

[6]Nuclear chemistry, atmospheric chemistry, and chemical education are treated somewhat more briefly within this chapter, as compared to other areas of chemistry due to their initial identification as subareas and only subsequent expansion.

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of current excitement, activity and importance and because they overlap across other fields of chemistry and science. They do not represent the complete breadth and vitality of analytical chemistry. Many of the other topics evaluated in this report overlap with analytical chemistry—for instance, nanoscience, computational chemistry, and spectroscopy.

Single-cell analysis is emerging as a field that will be critical to reaching a systems-level understanding of biological processes. Complete, preferably digital, information about the molecular states of individual cells is one aspect. Being able to observe even single molecules directly in context inside cells is a related goal. A further important aspect is the observation of interacting macromolecules in individual cells.

Sensors and detectors include the development and application of techniques and methods for sensing targeted chemicals or for broadband detection of many chemicals in vivo and in the environment.

Proteomics is a rapidly expanding field whose aim is to systematically study protein structure, function, interactions, and dynamics. Much effort is presently directed at the development of analytical strategies to analyze many proteins simultaneously. This developing technology is also influencing the design of critical medical studies and questions in biochemistry and bioorganic chemistry.

Molecular imaging includes mapping of specific chemicals and chemical properties across heterogeneous surfaces, such as lipids across cell surfaces, proteins atop tissue slices, and carbonyl grouping on carbon surfaces. Surface imaging includes exploration of topology and surface features in addition to chemical composition.

Microfluidics and miniaturization include the development of small and microscale devices to permit chemical measurements, with the objective of field portability or bedside use. Examples include Raman spectroscopy and mass spectrometry. The category also includes devices that employ small-scale fluidics to provide automated sample processing, chemical reactions, separation, and measurement in devices popularly called lab-on-a-chip.

Assessment

Analysis of the virtual congresses, highly cited papers, and the U.S. share of papers published in *Analytical Chemistry* (the leading journal for this area) as a whole, shows that the United States is the leader in analytical chemistry. The percentage of papers in *Analytical Chemistry* from non-U.S.

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chemists averaged 48 percent over 2000-2005. U.S. authors contributed an average of 41 percent of the papers in the three leading proteomics journals. These percentages support the suggestion that the United States holds a lower position in proteomics and in fact is several years behind Europe in this 11-year-old field.

Among the hot papers analyzed, 10 percent were attributed to analytical chemistry (Table 3-3); 60 percent of these articles were U.S. authored, 25 percent were from Western Europe, 5 percent were from Japan, 5 percent were from "other" Asia, and 5 percent were from all other countries or regions. These data taken alone would place the U.S. as the leader in analytical chemistry. In terms of journal citations, contributions to highly cited articles from the area of analytical chemistry have grown over the years—from 37.5 percent for 1990-1994 and 48.8 percent for 1995-1999, to 49.3 percent for 2000-2006. Taken alone these data place the U.S. among the leaders in analytical chemistry. However, the U.S. contribution to the most cited articles in the ACS journal *Analytical Chemistry* has been declining, while Western Europe's contribution has increased significantly. U.S. authors contributed 75 percent of the most accessed articles in *Analytical Chemistry* and 70 percent in the *Journal of Proteomic Research*.

Many organizers of virtual congresses in analytical chemistry further divided and defined the five subareas. In molecular and surface imaging, microfluidics and miniaturization, and sensors and detection, 63 to 66 percent of the speakers were U.S. scientists. In single-cell analysis, where only U.S. organizers responded, 76 percent of the speakers nominated were from the United States. In proteomics, where the majority of responding organizers were non-U.S., 47 percent of the speakers proposed were U.S. scientists. From these results it appears that U.S. scientists make up at least half of the leaders in these fields of analytical chemistry.

The combination of all the data from publications analyses and virtual congress results point to the U.S. being the leader in analytical chemistry.

The United States Is Among the Leaders in Atmospheric Chemistry

Atmospheric chemistry is an interdisciplinary field that deals with chemical composition, transformation, and transport in the atmosphere. Understanding chemical sources, their inputs, and their transport and transformation is a major goal of atmospheric chemistry. The three major subfields of atmospheric chemistryare: 1) field measurements, 2) modeling, and 3) laboratory studies. There is synergistic interplay between these three areas. An aim of the field measurements area is to measure the abundance of chemical pollutants and their sources in the atmosphere. Field studies also give a direct measure of the transport of chemical species throughout the atmosphere. The modeling area aims to understand the fate and trans-

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port of pollutants. Modeling aims to provide a fundamental evaluation and test of our understanding of the underlying chemistry from laboratory studies to explain the chemical transformation and transport observed from field measurements. Models use fundamental information from laboratory chemical kinetic and mechanistic studies in all phases—gases, liquids, and solids—with photochemical transformation properties of chemical systems from laboratory studies to make predictions. Instruments to measure pollutant concentration and other characteristics are developed and tested in the laboratory and then deployed in the field. Laboratory studies use state-of-the-art tools from physical chemistry to provide accurate measurements of the chemical kinetics of reacting chemical entities and to develop a complete picture of the chemical transformation through reactive collisions and photochemistry.

To assess the current U.S. position in the field of atmospheric chemistry, the three areas of field measurement, modeling, and laboratory studies were examined.

Assessment

The United States is the leader in atmospheric chemistry as shown by the virtual congresses, which had 60 percent participants from the United States, where 75 percent of the participants from U.S. organizers were from the United States, and 52 percent of speakers from non-U.S. organizers were from the United States. The virtual congresses also showed a balance in representation from researchers involved in field measurement, laboratory, and modeling. From the virtual congress data, the laboratory measurement groups in the United States are the leaders in atmospheric chemistry. Over 80 percent of the participants from both U.S. and non-U.S. organizers were from the United States. Strong competition in the field measurement and modeling areas is coming from Germany and the United Kingdom. The virtual congress data taken alone place the U.S. as the leader in atmospheric chemistry.

In one of the premier journals that publish field measurement, modeling, and laboratory studies, the *Journal of Geophysical Research*, over the time period from 1997 to 2005, 63 percent of the papers were contributions from U.S. authors. Of the non-U.S.-authored contributions, 84 percent were from Europeans. During the time period of 1996-2006, U.S. authors contributed 45 percent of the 350 most highly cited articles to the *Journal of Geophysical Research*. Outside the European Union, China showed a steady rate of growth in contribution to the *Journal of Geophysical Research*. Two specialized journals in the field, the *Journal of Atmospheric Chemistry* and *Atmospheric Environment*, which publish a proportionally larger number of modeling and field measurement studies, indicate that the

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strongest competition is coming from Germany. For example, in the *Journal of Atmospheric Chemistry* the U.S. contribution in 2000 was 32 percent and that from Germany was 30 percent. In 2005, the U.S. contribution was 29 percent and that from Germany was 22 percent. Furthermore, the U.S. author contribution accounted for 17 percent of the 283 most highly cited articles from 1996 to 2006 in the *Journal of Atmospheric Chemistry*. Other active countries—France, the United Kingdom, and Japan—accounted for the difference. Other important journals where many laboratory studies are often published are the *Journal of Physical Chemistry* and *Chemical Physics*. Atmospheric chemistry contributions are highly consolidated with the physical chemistry experimental contributions, and no reliable information or inference could be obtained. The highly cited articles and other publication analysis places the U.S. among the leaders or lagging behind the leaders in the area of atmospheric chemistry.

The United States Is the Leader in Biological Chemistry

Biological chemistry involves the use of chemistry to develop a better understanding of biological processes. To assess the current status of the U.S. contribution to biological chemistry, five subareas were examined:

Chemical and structural biology is concerned with the development of chemical and biological approaches to solving problems in living systems, which usually involve determination of the three-dimensional structures of biomolecules, mainly proteins and nucleic acids, and their complexes with ligands, receptors, drugs, or other interacting components. The structural information provides a basis for understanding the mechanism and function of the biomolecules and for molecular design.

Biocatalysis is the study of biological catalysts with regard to their kinetics, mechanisms, specificity, and application in synthesis and analysis. In addition to the traditional study of mechanistic enzymology, biocatalysis is concerned with the use of recombinant DNA technology, site-specific mutagenesis, directed evolution, pathway engineering, substrate design, and structure-based approaches as tools for the development of novel catalysts and reactions.

Nucleic acids and functional genomics cover the chemistry and biology of gene-related substances. Current subjects of study include genomic sequencing, genotyping, and genomic profiling with arrays; DNA damage; and the functional study of genes, including, for example, the study of transcriptional and translational processes that translate into cellular function at the protein level.

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Signaling pathways is a subarea of biological chemistry that is concerned with the study of molecular interactions and/or reactions in sequence in the living system that triggers a functional event.

In vivo molecular imaging refers to the spatial and/or temporal visualization of different cellular elements and biochemical reactions in a living organism using different imaging methodologies and labeled tracers with high molecular specificity. Tracers are labeled with radioisotopes for nuclear imaging, (with positron emission tomography (PET), microPET and single photon emission computed tomography), fluorescent probes for optical imaging or paramagnetic ions for nuclear magnetic resonance (NMR) imaging.

Assessment

The United States is the leader in biological chemistry, especially with regard to innovative research in the areas of chemical and structural biology, signaling pathways, nucleic acids, and functional genomics, and is among the leaders in biocatalysis and in vivo molecular imaging.

In more specialized journals, U.S. authors contributed 60 percent to *Biochemistry*, 56 percent to *Protein Science*, 47 percent to *Bioconjugate Chemistry*, 45 percent to *Proteins*, 42 percent to *Nature Biotechnology*, 59 percent to the *Journal of Biological Chemistry*, 22 percent to *ChemBioChem*, 65 percent to *Nature Structure & Molecular Biology*, 45 percent to the *Journal of Molecular Biology,* and 62 percent to *Chemistry and Biology*. Taken alone, these data place the U.S. as the leader or among the leaders in biological chemistry.

Of the highly cited journal articles in biological chemistry, 55.9 percent were authored by U.S. scientists during 1990-1994, 57.4 percent during 1995-1999, and 54.4 percent during 2000-2006. The journal *Biochemistry* had 78 percent of its most accessed articles authored in the United States (2004-2005).

The virtual congresses in chemical and structural biology and nucleic acids and functional genomics had very high representation from U.S. participants, with 75 and 83 percent, respectively, of selected speakers from the United States. The virtual congresses in signaling pathways and in vivo imaging also had high representation from the United States, with 69 and 63 percent respectively. The subarea of biocatalysis had 49 percent of selected speakers from the United States. The virtual congresses also showed strength in chemical and structural biology for the United Kingdom and Germany; strength in nucleic acids and functional genomics for the Netherlands; and great strength in biocatalysis for Japan, the United Kingdom, and the Netherlands.

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When all the data for the area of biological chemistry are evaluated in concert, the results point to the U.S. as the leader in biological chemistry.

The United States Is the Leader in Chemistry Education

Chemistry education is a relatively new research area at the crossroads between chemistry and science education. The questions investigated often develop from concerns raised by teaching chemists, and the research tools come from the science education community. Chemical educators apply theories of teaching or learning to study the interaction between how students learn chemistry and how the subject is taught. A new paradigm where teaching innovations are introduced based on research is replacing the reverse process. Many of the papers in chemistry education still follow the old paradigm: evaluation of one teaching method versus another with little or no reference to the underlying learning theory or presentation of isolated bits of information on the teaching/learning process. Chemistry education researchers are hampered by their relative isolation since few universities have more than one chemistry educator.

The United States provides significant funding for education efforts in chemistry, but little funding is directed specifically at research in chemistry education. For example, NSF's Integrative Graduate Education and Research Traineeship Program involves large numbers of research chemists in education projects but does *not* focus on the research aspect of chemistry education.

Assessment

Publications by U.S. authors accounted for 64 percent of content for the *Journal of Chemical Education*, with the rest of papers being contributed mainly from Canada, the United Kingdom, and Spain. Other countries showing particular leadership and strength in this area are Australia, the Netherlands, Germany, and the United Kingdom. U.S. chemists contributed 74 percent of the highly cited articles in chemistry education between 1995 and 1999 and 68 percent between 2000 and 2006. These results taken alone place the U.S as the leader in chemical education. In the United States there are two chemistry education programs that have a concentration of researchers. These two programs (Purdue University and the University of Wisconsin) showed high visibility in the virtual congresses organized by non-U.S. chemical educators.

The virtual congress data show a 49 percent participation by U.S. speakers. When combined, the publications analysis and the virtual congress data place the U.S. as the leader in chemical education.

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The United States Is the Leader in Inorganic Chemistry

Inorganic chemistry deals with the chemistry of the elements of the entire Periodic Table. This includes synthesis, characterization, and theoretical studies. The field experienced a renaissance beginning in the 1950s, driven by appreciation of the diverse modes of reactivity and bonding as well as numerous industrial applications spanning many fields. To assess current U.S. vitality in the field of inorganic chemistry, four representative subareas of inorganic chemistry were analyzed:

Organometallic chemistry and homogeneous catalysis deal with the synthesis and transformations of compounds, or of transformations mediated by compounds, having metal-carbon and related metal-element bonds. Organometallic chemists carry out research on the synthesis, reactivity, and physical properties of organometallic compounds with a focus on unusual bonding situations, unusual transformations and their mechanisms, and theory to understand these phenomena. Homogeneous catalysis specialists strive to use these concepts to effect rapid and selective catalytic transformations. Organometallic compounds play an important role in both stoichiometric and catalytic organic synthesis, including routes to fine chemicals, pharmaceuticals, flavors and fragrances, and myriad industrial chemicals. Other important uses of organometallic compounds are as precursors of diverse electronic and optoelectronic materials. This includes the synthesis of compounds important in the production of computer logic and display components, solid state lasers, and cell phone components, primarily via chemical vapor deposition film growth processes.

Main group chemistry focuses on elements other than carbon and transition metals. While much attention is paid to unusual bonding situations, unusual reactivity, and the theory to understand these phenomena, the importance of main group chemistry also lies in its application to other areas. Main group compounds (frequently organometallic compounds) play a major role in synthetic organic chemistry, with examples being boron (B) for hydroboration, catalytic Suzuki coupling, lithium (Li) and magnesium (Mg) as alkylating reagents, aluminum (Al) for reductions, silicon (Si) for protecting groups, tin (Sn) for catalytic coupling reactions, and sulfur (S) and selenium (Se) for selective oxidations.

Another major application for main group chemistry is in solid state chemistry relevant to electronic and optoelectronic materials. Ultrapure Si is the basis of almost all computer logic and display components, and the production and processing of these materials rely heavily on highly optimized Si and in some cases, germanium (Ge), reaction chemistry. Likewise, the III-V materials produced for solid state lasers and cell phone components rely

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heavily on the ability to manipulate gallium (Ga), indium (In), arsenic (As), and antimony (Sb) compounds in chemical vapor deposition processes.

In the materials as well as biomaterials areas, Si and Al compounds are produced on a large scale for catalyst supports, solid phases for chromatographic and gas separations, sorbants, silicone fluids and resins, silicones for artificial organs/veins, and so forth. Fluorocarbons find use in high-performance polymers such as Teflon and Nafion. In the biomedical area, B compounds are used for neutron-capture therapy, barium (Ba) compounds for X-ray imaging, lanthanide compounds for magnetic resonance imaging, and fluorinated organic molecules in numerous pharmaceuticals.

Bioinorganic chemistry deals primarily with the role of metal ions in biology. Today, the great bulk of traditional coordination chemistry research has merged with bioinorganic chemistry, and this area spans the gamut from understanding the roles of metal ions in metalloenzyme function to new metal-containing drugs and imaging agents. Contemporary bioinorganic research involves both the synthesis and understanding of "model compounds" that serve as instructive functional or spectroscopic facsimiles of metalloenzyme active sites to detailed studies of wild and modified biological systems. Key questions concern how Nature has modified metal ion environments to allow enzymatic functions often difficult or impossible to achieve in simple synthetic complexes, such as molecular oxygen binding and activation, reduction and functionalization of molecular nitrogen, selective hydrocarbon functionalization, photosynthesis, and protein shape control. Beyond metalloenzymes, metal-based pharmaceuticals play an important role as antitumor agents and other drugs. Bioinorganic chemists also study new types of imaging agents both for diagnostics and to understand drug action mechanisms; examples include lanthanides (MRI) and radiopharmaceuticals such as technetium (Tc).

Solid state chemistry includes the synthesis, characterization, and application of extended oxide, chalcogenide, halide, carbide, nitride, and other solids. The elemental constituents in solid state chemistry span the entire Periodic Table, and the research focus is likewise very broad. Solid state chemists study new synthetic methods (many exotic by molecular chemistry standards), diverse characterization methods (many at the frontier of chemistry and solid state physics), theory appropriate for extended solids, and the applications of solid state compounds. The latter is vast, ranging from cement and ceramics for fabrication of large, high-strength object, to materials for magnets, data storage, lasers, optical detectors, photovoltaic cells, catalysts, supports for separations, turbines, catalysts, artificial bones, conductors, semiconductors, superconductors, batteries, X-ray detectors, emissive displays, cutting tools, and coatings of all sorts.

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Assessment

The virtual congresses in organometallic chemistry and homogeneous catalysis had 50 percent of the chosen speakers from the United States. The virtual congress data also showed strength in organometallic chemistry and homogeneous catalysis for Germany, Japan, Canada, the Netherlands, and Spain. In this area, the United States has strong competition in Europe and Asia. For example, recent Nobel prizes have been given jointly to investigators from the United States and Japan and from the United States and France. U.S. authors contributed 26 percent of the papers to the journal *Organometallics* and 55 percent of the 40 most accessed papers in 2004-2005 (major international contributions came from Italy, the United Kingdom, Germany, Spain, and Japan).

The United States is among the leaders in main group chemistry. In the virtual congress assessment, only 39 percent of the chosen speakers were U.S. chemists; Germany, Japan, the United Kingdom, Canada, and France showed strength. While no ACS journal is devoted exclusively to main group chemistry, U.S. contributions to *Inorganic Chemistry* and *Organometallics* (which have significant main group representations) are 35 percent and 26 percent, respectively.

The United States is clearly the leader in bioinorganic chemistry. In the virtual congress assessment, 71 percent of the chosen speakers were from the United States; speakers from Germany, Japan, the United Kingdom, Italy, and Spain also were also prominent. While no ACS journal is devoted exclusively to bioinorganic chemistry, *Inorganic Chemistry* publishes many bioinorganic papers and U.S. authors accounted for 35 percent of the papers in *Inorganic Chemistry* and for 60 percent of the papers in *Biochemistry*. U.S. bioinorganic chemistry is successful because it is well supported by National Institutes of Health funding and because U.S. chemists perceive that it deals with timely and important problems. Consequently, bioinorganic chemistry attracts talented faculty and students and enjoys excellent support in terms of facilities, instrumentation, and training grants.

The United States is the leader in solid state chemistry. U.S. speakers have 57 percent representation at both the virtual congresses and specialized Gordon Research Conferences. The leaders, particularly in materials synthesis, are France, Germany, the United Kingdom, and Japan; U.S. students often choose to pursue postdoctoral studies in materials synthesis in these countries. High-pressure crystal growth facilities, which are critical for research in this subfield, are lacking in the United States, but many exist in Japan and Russia.

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The United States Is the Leader or Among the Leaders in Macromolecular Chemistry

Macromolecular chemistry (a more modern and inclusive name than polymer chemistry) involves the synthesis and physical characterization of high molecular weight (> 2,000 g/mol) organic or inorganic materials having well-defined repeating units. Early research in macromolecular chemistry originated from industrial and military laboratories dealing with synthetic plastics. However, this discipline has emerged as an interdisciplinary field ranging from petroleum-based macromolecules to biological macromolecules, including nucleic acids, proteins, and polysaccharides. Macromolecular chemistry is an enabling science that impacts diverse technologies, including energy and sustainability, biomedicine, electronics, and structural materials.

The impact of macromolecular chemistry on our nation's commercial, military, and scientific competitiveness is extraordinary. Macromolecular chemistry provides materials for automobiles and diverse consumer applications, including drug delivery and biomaterials. Macromolecules are used in clothing fibers, computers, semiconductor imaging, cosmetics, structural films and sheets, food and beverage packaging, adhesives, artificial organs, tissue scaffolds, surgical sutures, and automobile parts. During the past decade, macromolecules have played critical roles in the development of new technologies such as nanotechnology, biomedical devices, alternative energy technologies, photovoltaic devices, membranes, sensors, fuel cell components, and smart and self-healing coatings.

Supramolecular chemistry is an emerging subarea that focuses on assemblies of covalent molecules held together by noncovalent bonding interactions. Supramolecular chemistry utilizes far weaker and reversible noncovalent interactions, such as hydrogen bonding, metal coordination, hydrophobic forces, and electrostatic effects to assemble molecules into multimolecular complexes. Important concepts that have been demonstrated by supramolecular chemistry include host-guest chemistry, self-assembly, and molecular recognition. Supramolecular chemistry is often deeply integrated within the macromolecular chemistry field as researchers are now using tailored intermolecular interactions for the construction of a repeating unit.

To assess the current status of the U.S. contribution to macromolecular chemistry, four representative subareas were examined:

Macromolecular synthesis involves the design of synthetic methodology for the formation of macromolecular architecture, including controlled molecular weight and molecular weight distribution, stereochemistry, topology (linear, branched, and cross-linked), block and graft copolymers, and

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hyperbranched/dendritic structures. Biomacromolecular chemistry deals with bioderived monomers, macromolecular interactions with biological structures, biomaterials, biodegradation, drug/gene delivery, macromolecular interactions at the cellular level, and in vivo applications. There is a synergy between advances in macromolecular synthesis and advances in structural characterization by nuclear magnetic resonance and in situ Fourier transform infrared FTIR spectroscopy, size exclusion chromatography, and mass spectrometry.

Supramolecular chemistry uses tailored noncovalent bonding for the rational design of macromolecular architectures. Multihydrogen bonding, self-assembly, electrostatic interactions, amphiphilic organization, and metal-ligand interactions are utilized for the formation of potentially reversible macromolecular architecture. An emerging area involves the integration of biological structures that inspire sophisticated molecular recognition events with synthetic scaffolds.

Physical characterization of macromolecular systems strives to determine chemical structure/property relationships. This subfield includes study of thermomechanical performance; viscoelastic properties; surface properties, adhesion science; thermal transitions; morphological analysis, including semicrystalline, amorphous, liquid-crystalline, and microphase-separated structures. Structural analysis employs electron microscopy, confocal microscopy, optical microscopy, x-ray photoelectron spectroscopy, atomic force microscopy, and x-ray and neutron scattering of macromolecular compositions.

Rheology (the study of deformation and flow of materials) provides the fundamental understanding needed to develop technologies for processing macromolecular materials to fabricate coatings, films, molded objects, and fibers. Research efforts strive to correlate macromolecular structure with viscosity (melt and solution) and modulus (stiffness) as a function of frequency and temperature. Polymer physics and molecular modeling of macromolecular structure and diffusion are fundamental to advances in this field.

Assessment

The United States is the leader in most areas of macromolecular chemistry, as shown by virtual congress data. The virtual congresses in macromolecular synthesis had a very high, 64 percent, representation from U.S. speakers. Those on the physical characterization of macromolecules also showed a very high 68 percent proportion of U.S. speakers (this number

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may be inflated since only U.S. organizers responded). The virtual congresses in processing and rheology had a strong 50 percent representation from U.S. speakers. The supramolecular chemistry congresses had only 39 percent U.S. speakers. The United States was certainly not dominant in this important emerging field and intense competition from Europe was evident.

Analysis of hot papers (May-June 2006) showed that macromolecular chemistry accounted for 8 percent in chemistry and that U.S. chemists authored 46 percent of these macromolecular chemistry papers. The United States showed leadership in the areas of macromolecular synthesis and physical characterization and solid state structure with 75 percent of the hot papers. None of the hot papers in supramolecular chemistry came from U.S. authors; Western Europe showed leadership in this area with 40 percent of the hot papers.

Analysis of Thomson ISI data on the most highly cited papers in macromolecular chemistry journals showed a strong but declining contribution from U.S. authors, who accounted for 46 percent of the most highly cited papers from 1990 to 1994 and 35 percent from 2000 to 2006. International competition from Japan, Europe and China appears to be rising.

Macromolecules research accounted for 8.2 percent of all hot papers in chemistry from 2004 to 2006. Of these papers, 46.2 percent were contributed by the United States, 15.4 percent byWestern Europe, 15.4 percent by Japan, 7.7 percent by Asia (other), and 15.4 percent by all other. Only one-third of the most accessed ACS articles from the journal *Biomacromolecules* were contributed by U.S. scientists. In the journal *Macromolecules*, 48 percent of the most accessed ACS articles were contributed by U.S. scientists.

The leadership of U.S. macromolecular chemists was also demonstrated by their strong overall contributions (33 percent) to the ACS journal *Macromolecules*. This journal is traditionally more oriented toward physical property measurements and less toward macromolecular synthesis. It is important to note that U.S. authorship in *Macromolecules* was down significantly from 51 percent from 1990 to 94, showing a significant increase in international competition, although the United States remains a leader. Authorship of papers in *Macromolecules* indicates rising competition from Germany, Japan, and more recently China (7 percent of publications and 20 percent of the most accessed articles from 2004-2005). There is significant focus on macromolecular materials and electronic materials in Asia and Japan, where chemists are looking for the performance of macromolecules to enable new technologies.

Langmuir, the ACS journal covering the areas of colloids, surfaces, and interfaces, also showed a strong contribution from U.S. authors (35 percent of all papers and 68 percent of the 40 most accessed papers for 2004-

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2005); authors from Japan, Germany, the United Kingdom, and China also were major contributors. In the ACS journal *Chemistry of Materials*, U.S. authors were the leading contributors (30 percent of all papers and 40 percent of the most accessed papers for 2004-2005); authors from Japan, Germany, France, and China were also major contributors. U.S. authorship in the relatively new ACS journal *Biomacromolecules*, with editorial offices based in Europe, was 25 percent of all papers and 23 percent of the 40 most accessed papers for 2004-2005). U.S. authorship in the United Kingdom journal *Polymer* remained stable at 20 to 25 percent over the past decade, and 50 percent of the 30 most cited papers in *Polymer* were from U.S. authors.

Based on the overall publications record in top journals and authorship of highly cited and hot papers, combined with the virtual congress results, the U.S. is the leader or is among the leaders in macromolecular chemistry.

The United States Is the Leader in Materials Chemistry and Nanoscience

The field of materials chemistry and nanoscience builds the bridge between fundamental chemistry and applied science and technology. The synthesis of materials, the improvement of their physicochemical properties, the development of reliable processing and fabrication routes leading to miniaturization, and the design of "smart" structures and devices are pivotal to industrial growth and a competitive economy.

The expertise required to tackle these diverse materials problems is largely provided by chemists. However, due to the highly multidisciplinary nature of the field, researchers work across a variety of disciplines (chemistry, physics, engineering, materials science, biology), and synergistic interactions among scientists from different disciplines are often required to create productive environments for interdisciplinary research collaboration. Even the chemistry field, there is a strong overlap between materials chemistry and physical, polymer, inorganic, and computational chemistry. It is noteworthy that the field of materials chemistry and nanoscience is the fastest developing field in chemistry: While the total number of articles in chemistry steadily increased by about 25 percent every five years, the number of papers in nanochemistry increased exponentially—by 150 percent from 1995 to 2000 and by another 250 percent from 2000 to 2005.

To assess the current status of the U.S. contribution to modern materials and nanochemistry, six representative subareas were identified:

Self-assembly science addresses the chemical, biochemical, and physical aspects of the ability of molecules, particles, and systems to assemble into higher-order structures. The subfield is very diverse, with "hot" topics

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including self-assembled monolayers and multilayers, hierarchical assembly, assembly of nanoparticles, liquid crystals, supramolecular assembly, surfactant-driven assembly, assembly of biomolecules (DNA, proteins, etc.), polymer assembly, control of the assembly of dissimilar materials into hybrid structures, multicomponent assembly, synthetic membranes and vesicles, and computer modeling of self-assembled systems.

Nanocrystal and cluster science is the study of the chemical synthesis and physical properties of individual nanocrystals and nanotubes. It seeks to understand the evolution of molecular properties into solid state properties with increasing size. Methods include so-called bottom-up chemical synthesis of nanocrystals, nanowires, and very large species, as well as physical molecular beam approaches. Advanced physical characterization of single nano-objects by local probe methods and optics is critical here. The area is intrinsically interdisciplinary at the junction of physics, chemistry, and materials science. Outstanding chemical research in nanocrystal science is often found in a wide variety of science and engineering departments.

Nanomaterials: energy and applications: As nanocrystals and nanotubes are better understood, it becomes possible to rationally design nanostructured materials for specific purposes. This area includes both chemical synthesis and physical properties of nanostructured materials incorporating fullerenes, organic conductive polymers, and inorganic nanostructures. A central goal is composite materials for solar energy utilization—new types of solar cells.

Biomaterials/bio-inspired materials synthesis: The general objective of this new, and rapidly developing subfield is to search for smart biological solutions in the synthesis, assembly, and integration of complex materials systems and to apply this knowledge to develop biomimetic synthetic strategies with the ultimate goal of creating new materials of technical importance. The hot topics in the subfield encompass the assessment of materials properties (optical, electronic, mechanical, nanostructural) of exquisite biogenic structures; the characterization of biomacromolecules that control their formation; biomineralization mechanisms; the study of templating at the organic/inorganic interfaces; bottom-up synthetic strategies; harnessing the potential of biomolecules or organisms for the synthesis and assembly of artificial materials with advanced properties; the use of biological strategies in a different environment to create new materials but without biological fragility; and "smart," responsive materials.

Bionano is an emerging interdisciplinary area that studies biological and hybrid biological/synthetic nanostructures. Chemical aspects of this

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subfield include the synthesis and extraction of bionanocomponents; the assembly/bonding of biological nanostructures without loss of functionality; the integration and linking of biologically derived nanostructures (e.g., proteins, lipids, nucleic acids, carbohydrates) with any physically or chemicallynanofabricated components (e.g., carbon nanotubes, nanolithographed parts, fluorophores), to introduce fields, information transduction, or other functionality; the study of the physicochemical properties of hybrid bionanostructures with tailored interactions and functionality; and the development of computational approaches to predict and rationally design various functional bionanostructures.

Tissue engineering/biocompatibility is a highly multidisciplinary area that represents the confluence of three quite different domains—clinical medicine, engineering, and science—addressing the development of materials that restore, maintain, or improve tissue function. Chemical and biochemical research plays an increasingly important role in this area. Critical topics include chemical modification of natural materials for use in medicine, synthesis of artificial implant materials for bone repair and artificial organs, development of biocompatible and biodegradable polymeric and ceramic materials, and creating biocompatible surface chemistries for integrating synthetic materials into living tissue. There is a strong overlap between this subfield and polymer chemistry, ceramics, and surface chemistry.

The materials aspects of organic electronics, polymers, and solid state chemistry are described in the physical chemistry, macromolecular chemistry, and inorganic chemistry fields, respectively.

Assessment

The United States is the leader in materials chemistry and nanoscience in general. Its position varies, however, within different subareas, ranging from strong leadership to being among the leaders in specific subfields.

The United States has a very strong, perhaps even dominant position in nanocrystal and cluster science, as shown by virtual congress results: U.S. congress organizers had 75 percent U.S. speakers, and non-U.S. organizers had 50 percent U.S. speakers. The United States is the strong leader in the subfields of bionano and tissue engineering/biocompatibility, with very high (about 80 percent) representation from U.S. virtual speakers proposed by both U.S. and non-U.S. virtual congress organizers. The United States is the leader but not the dominant force in the subfields of self-assembly science and biomaterials/bio-inspired materials synthesis: U.S. congress organizers had 78 and 60 percent of U.S. speakers for the two subfields, respectively, while non-

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U.S. organizers had 48 and 47 percent of U.S. speakers. When taken alone, the virtual congress data suggest that the U.S. is the leader in nanoscience.

The virtual congress data also revealed strong competition in self-assembly science from Europe (particularly from France, due to 1987 Nobel Prize laureate Jean-Marie Lehn and researchers trained in his group), Israel, and Japan. In biomaterials/bio-inspired materials synthesis, other countries that showed great strength were Israel, Germany, and the United Kingdom. There are significant research efforts in bionano in Europe (Switzerland, the United Kingdom, and Germany, in particular). In tissue engineering/biocompatibility there is competition from Switzerland, Japan, and Canada.

U.S. leadership is also demonstrated by contributions to the top peer-reviewed journals in materials chemistry and nanoscience. The new ACS journal *Nano Letters* presently has the highest impact factor of all ACS journals. It draws papers from a wide variety of academic departments and from strong overseas groups. The strong position of U.S. chemistry in the nanoscience area is shown by the U.S. scientists' contribution of 66 percent of the papers and 82.5 percent of most accessed articles in *Nano Letters*. The contribution of U.S. authors was 43, 38, 32, 35, and 30 percent in *Nature Materials*, *Advanced Materials*, *Advanced Functional Materials*, *Langmuir*, and *Chemistry of Materials*, respectively. U.S. representation in the top 40 most accessed articles published in 2004-2005 in *Langmuir* and *Chemistry of Materials* was 50 percent in each journal. In materials chemistry, U.S. scientists contributed 41 percent of the most highly-cited articles from 2000 to 2006. Materials/nanoscience is the largest hot area in chemistry, accounting for 37 percent of all the hot articles 2004 to 2006. U.S. authors contributed 60 percent of the hot articles, and Western European authors contributed 28 percent. Based on the total authorship of most cited and hot papers, the U.S. is the leader in the field of nanoscience.

The leading position of the United States in materials chemistry and nanoscience was recognized by the Nobel Prize given to Richard Smalley and Robert Curl and by the Kyoto Prize awarded to George Whitesides.

The extreme multidisciplinary aspect of nanoscience is an ingredient of the U.S. success. U.S. academic training is typically broader than European and Japanese training in chemistry, and specialization occurs later in U.S. training. U.S. researchers are more able to assimilate and apply basic knowledge from different academic areas. Another reason for the leadership position is the strong new funding in nanoscience from the federal government.

The United States Is Among or Lagging Behind the Leaders in Nuclear and Radiochemistry

Nuclear and radiochemistry deals with radioactive substances—from fundamental studies of atomic nuclei and chemical properties of radioactive elements to practical applications of radioactivity and nuclear technology.

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Nuclear and radiochemistry includes accelerator/reactor chemistry for isotope production, nuclear structure, neutrino chemistry, nuclear forensics, and archeometery. Understanding of nuclear and radiochemistry underlies the availability of adequate supplies as well as proper and safe use of radioactivity for energy production or radiomedicine. Twenty percent of electric power in the United States is supplied by nuclear reactors. It is possible that construction of new reactors in the United States will resume within the next decade. Similarly, the use of radionuclides in medicine, research, and industry is predicted to increase.

In assessing the current status of the U.S. contribution to nuclear and radiochemistry, several subareas were considered:

Basic nuclear science includes the synthesis of radionuclides, production of new elements, generation of radioactive and exotic nuclear beams, determination of nuclear properties, and applications of nuclear spectroscopy.

The subarea of nuclear energy production and nuclear waste concerns include studies of fuel cycles for Gen IV and Post Gen IV reactors, environmental studies of radioactive wastes, studies of the effects of radiation on fuel materials and wastes, and transmutation of radioactive waste products to reduce their lifetimes.

Environmental behavior of actinides includes studies of actinide interactions related to geochemistry; actinide interactions with microbes; and actinide redox reactions, speciation, and complexation.

Nuclear forensics involves using nuclear signatures to define the origin of radioactive materials, stable isotope signatures to determine geolocation, and conventional forensic information (fingerprints and fibers) from radiological samples.

Nuclear neutrino research includes neutrino experiments such as SNO, Super-Kamiokande, KamLAND, SAGE, and double-beta decay and theory of neutrino oscillations.

Nuclear isotope production involves policy studies of facilities for research and development of isotope production, radiochemistry education, and the role of national laboratories in isotope R&D.

Assessment

The United States has been recognized as a leader in nuclear and radiochemistry since the end of World War II. However, this leadership is eroding. Most of the research in nuclear and radiochemistry in the United

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States is carried out at national laboratories. The number of U.S. chemistry departments offering a specialization in nuclear chemistry has decreased continuously over the past 30 years. There has been a corresponding sharp decline in the numbers of Ph.D.s in nuclear and radiochemistry (23 U.S. Ph.D.s from 1970 to 1980 versus 12 Ph.D.s from 1990 to 2000). According to the 2005 ACS Directory of Graduate Research, only a dozen departments still have a program in nuclear chemistry and these typically have one or two active faculty members.

The virtual congresses in nuclear chemistry were conducted a bit differently because of the smaller number of researchers in this community. Six individuals, all from the United States and five from national laboratories, were asked to develop a virtual congress in a different specialty area of nuclear chemistry. While the organizers were asked to pick about 20 congress participants, they provided an average of only 13 each. This is in contrast to many of the other areas of chemistry examined in this study, where most organizers had difficulty limiting themselves to only 20 names. Based on 52 percent representation from U.S. participants in the nuclear chemistry virtual congresses, the United States is considered the leader in this area. Other countries with significant representation are Germany, Japan, and the United Kingdom.

Based on journal analysis, the United States is among or lagging behind the leaders. In 2005, 19 percent of articles in *Radiochimica Acta*, approximately 30 percent in the *Journal of Radioanalytical Nuclear Chemistry*, and 30 percent in *Separation Science and Technology* were from U.S. authors. Authors from Japan and Western Europe, particularly Germany, are major contributors to these journals. Examination of the most cited articles in the *Journal of Radioanalytical Nuclear Chemistry* shows that the United States and Japan were the two largest single-country contributors (each with 10-20 percent of the authors), but Western Europe made the strongest regional contribution. Authors from Western Europe also contributed the greatest number of most cited articles to *Radiochimica Acta*, followed by authors from the United States and Japan.

Although the results from the virtual congress exercise show that the U.S. nuclear and radio chemists are still highly regarded, the declining number of U.S. nuclear and radiochemists, and the analysis of journal publications, all point to the United States being among the leaders or lagging behind the leaders in nuclear and radiochemistry.

The United States Is Among the Leaders in Organic Chemistry

Organic chemistry deals with all aspects of the chemistry of carbon compounds. Since carbon compounds, including fats, sugars, proteins, and nucleic acids, are the building blocks of all living organisms, there is

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a strong linkage between organic chemistry and the chemistry of life processes. Organic chemists design and synthesize drugs to improve human health, agricultural chemicals to safeguard the food supply, commodity chemicals for use as personal care products, and polymers for use as structural materials or fibers for clothing. Organic chemists design processes to convert petroleum, coal, and biomass to fuels for transportation and a myriad of materials that enhance our daily lives.

Because chemistry has become so multidisciplinary, there is strong overlap and synergy between organic chemistry and biochemistry, pharmaceutical sciences, macromolecular chemistry, materials chemistry, and inorganic chemistry. Organic chemists in turn rely on advances in analytical chemistry, physical chemistry, and computational chemistry.

To assess the current status of the U.S. contribution to organic chemistry, five representative subareas of organic chemistry were examined:

Synthetic organic chemistry involves developing efficient and selective new reactions and designing and implementing the synthesis of complex molecules, including those related to natural products.

Medicinal chemistry and drug discovery is a more applied but crucial subarea of organic chemistry. Medicinal chemists design and synthesize new organic compounds to test as drug candidates. They seek to understand and exploit the interaction of organic compounds with living organisms to develop new therapies.

Natural products chemistry involves the isolation of new materials from living organisms and determination of their structure and biological activity. Natural products chemistry often provides leads for new kinds of pharmaceutical activity.

Physical organic chemistry focuses on discovering the mechanisms of reactions and understanding the chemical and physical properties of organic molecules in molecular terms. The development of new synthetic methods often gets its inspiration from mechanistic studies or from biological chemistry.

Organocatalysis is the study of reactions that employ catalysts based solely on organic compounds. This is a recent area of intense interest and complements traditional catalysts based on transition metal complexes. Organometallic chemistry and homogeneous catalysis were discussed earlier as a subarea of inorganic chemistry. Increasingly chemists seek to find catalytic methods for synthesis.

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Assessment

The United States is among the leaders in most areas of organic chemistry. The virtual congresses in medicinal chemistry and drug discovery had a very high 69 percent representation from U.S. participants. Those in synthetic organic chemistry and physical organic chemistry had 60 percent of the chosen speakers from the United States. The virtual congresses in natural products chemistry, organocatalysis, and organometallic chemistry and homogeneous catalysis had 50 percent of the chosen speakers from the United States. Taken alone, the virtual congress data place the U.S. as the leader in organic chemistry.

The virtual congress data also showed strength in synthetic organic chemistry Japan, the United Kingdom, Germany, Switzerland, and the Netherlands; strength in medicinal chemistry and drug discovery in Germany, Switzerland, the United Kingdom, and France; strength in natural products chemistry in Japan, Germany, and Israel; strength in physical organic chemistry in Germany, Switzerland, the United Kingdom, and Japan; great strength in organocatalysis in Germany and Japan; and strength in organometallic chemistry and homogeneous catalysis in Germany, Japan, Canada, the Netherlands, and Spain.

Analysis of "hot papers" (May-June 2006) showed that organic chemistry had a strong representation with 52 of 200 papers and that U.S. authors contributed 32 percent of those papers. Synthetic organic chemistry with 46 hot papers (36 percent from U.S. authors and 45 percent from Western Europe) and organocatalysis with 24 papers (23 percent from U.S. authors and 58 percent from Western Europe) appear to be particularly hot areas. In addition, there were 31 hot papers (40 percent from U.S. authors and 40 percent from Western Europe) from the related area of organometallic chemistry and homogeneous catalysis. The hot papers analysis shows very strong competition from Western Europe. Taken alone, the data on hot papers places the United States among the leaders in organic chemistry.

Analysis of Thomson ISI data on the most highly cited papers in organic chemistry journals showed a strong but declining contribution from U.S. authors, who accounted for 59 percent of the most highly cited papers from 1990 to 1994 and 47 percent from 2000 to 2006. In the same period, contributions from Western Europe rose from 27 to 29 percent, those from Japan increased from 6 to 13 percent, and those from China and India tripled from 2 to 6 percent. This publications analysis places the United States among the leaders in organic chemistry.

It is important to mention that U.S. contributions were particularly strong to the outstanding organic publications of the *Journal of Organic Chemistry* (36 percent of all papers and 80 percent of the 40 most accessed papers from 2004 to 2005) and *Organic Letters* (41 percent of all papers

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and 62 percent of the 40 most accessed papers from 2004-2005). In both of these journals, international organic chemists increased their contributions in the past five years from 61 to 64 percent and from 53 to 59 percent, respectively. The most active countries were Japan, China, Spain, Germany, France, the United Kingdom, and Canada.

In more specialized journals, U.S. authors contributed 41 percent of the papers to the *Journal of Medicinal Chemistry* and 50 percent of the 40 most accessed papers from 2004 to 2005 (major international contributions from Italy, the United Kingdom, Germany, Spain, and Japan) and 22 percent of the papers to the *Journal of Natural Products* (major international contributions from Japan, China, Taiwan, Germany, Thailand, and Australia). Natural product discovery is often the first area to become strong in developing nations (often involving collaborations with Japan or European countries). The strong showing of U.S. and European Union chemists in medicinal chemistry reflects the strength of their countries' pharmaceutical industries.

The United States Is the Leader or Among the Leaders in Physical Chemistry

Physical chemistry focuses on identification of the molecular-scale events that constitute chemical reactions in all phases: gases, liquids, and solids. The chemical reaction may be initiated thermally, by photon absorption, by interaction with electrons, by collisions with high-energy particles, or by interaction with a solid or liquid surface. Experimental characterization of reactive events involves determining the energy levels of reactants, transition states, and products; the motions of the reactants, transition states, and products as the reaction proceeds; and the interactions of the reactants, transition states, and products with the surrounding molecules. The reactants, transition states, or products may be neutral species, positive or negative ions and may be as small as a hydrogen atom or as large as a protein molecule or a nanoparticle.

Physical chemists often uncover new processes that are then developed into techniques accessible to a wide range of scientists; an example is magnetic resonance imaging. Physical chemists also discover new species such as C_{60}, which opened the new subareas of nanoscience. Thus, there is strong overlap and synergy between physics, chemistry, and all other chemistry areas, particularly analytical chemistry, macromolecular chemistry, and materials chemistry. Many techniques with origins in physical chemistry are also employed in the disciplines of physics, biology, chemical and environmental engineering, geology, and medicine. Physical chemistry experiments most often provide data to which theoretical predictions and computational results are compared.

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To assess the current status of the U.S. contribution to physical chemistry, seven representative, but overlapping subareas of experimental physical chemistry were examined:

Biophysical chemistry is physical chemistry applied specifically to systems of biological interest. This effort is also pursued extensively in physics, biochemistry, and biology departments for the purpose of improved drug design and medical procedures.

Heterogeneous catalysis probes mechanisms of reactions that typically occur on metallic nanoclusters supported on insulators such as transition metal oxides. These studies relate directly to many commercial processes such as oil refining, hydrogen production, and food processing.

High-resolution spectroscopy primarily employs optical techniques in the frequency domain with the goal of identifying molecular energy levels. The energy level information forms the basis of a wide range of analytical techniques employed in environmental and atmospheric monitoring.

Reaction dynamics involves determination of the motions and energies of the reactants as they evolve through the transition state to the final products. A wide variety of optical, electronic, and scattering techniques are used to probe the dynamics of chemical reactions occurring in the gas, liquid, or solid phase as well as on surfaces. Such information is critical for designing more efficient reactions and processes in energy technology, drug production, and environmental cleanup.

Single-molecule imaging and electronics is the study of single molecules by optical and/or electronic methods, including both understanding of single-molecule or nanotube electronic devices, and microscope and laser-based optical methods to characterize single species in complex environments, often in a biological or medical context. This effort is being pursued vigorously in physics, chemistry, and biology departments; in medical research; and in industrial development of new DNA sequencing methods.

Surfaces and interfaces chemistry is the study of the structure and reactivity of liquid and solid surfaces. The surfaces may be extended or may be limited to the nanometer scale. The surface, often a transition metal, may be a catalyst for a chemical reaction. Such studies provide the fundamental principles of the commercially important area of heterogeneous catalysis, which is essential to fuel and metal production, food processing, and commodity chemical manufacturing. The surface may also be consumed as a reactant, such as in semiconductor etching. These studies provide the basic chemistry of the manufacturing of electronic components and devices.

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Ultrafast spectroscopy primarily employs optical techniques to study molecular motion in the femtosecond to attosecond range.

Assessment

The United States is the leader in all areas of physical chemistry, according to the results obtained for virtual conferences organized by U.S. scientists. In addition, the United States is among the leaders in the vast majority of areas. according to the results obtained for conferences organized by non-U.S. scientists. The virtual congress in biophysical chemistry had very high representation, 77 percent, by U.S. participants, for congresses organized by U.S. scientists and 46 percent representation by U.S. participants when organized by non-U.S. scientists. The U.S. representation in congresses in reaction dynamics, high-resolution spectroscopy, ultrafast spectroscopy, and surfaces/interfaces was between 60 and 69 percent when organized by U.S. scientists and between 36 and 49 percent when organized by non-U.S. scientists. U.S. representation in the heterogeneous catalysis virtual congress was 58 percent when organized by U.S. scientists and 24 percent when organized by non-U.S. scientists. The virtual congress in single-molecule imaging and electronics had 65 percent of the chosen speakers from the United States when organized by U.S. scientists and 70 percent of the speakers when organized by a single non-U.S. scientist.

The virtual congress data showed strength in biophysical chemistry for Germany, the United Kingdom, Japan, and Switzerland; strength in reaction dynamics and high-resolution spectroscopy for Taiwan, Germany, Switzerland, Italy, China, Canada, the Netherlands, and France; strength in ultrafast spectroscopy for Germany, Switzerland, Canada, the Netherlands, and France; strength in single-molecule imaging and electronics for Germany, Switzerland, the Netherlands, Japan, and Sweden; strength in surfaces/interfaces for Germany, Denmark, and Japan; and strength in heterogeneous catalysis for Germany, Japan, Denmark, the Netherlands, France, Switzerland, and Spain.

The leadership of U.S. physical chemists is also demonstrated by their strong overall contributions to the *Journal of Physical Chemistry A and B* (about 35 percent of all papers and an average of 75 percent of the 20 most accessed papers from 2004 to 2005). In these two journals, international physical chemists have increased their contributions in the past five years from 57 to 65 percent. The most active countries were Japan, China, Spain, Germany, Italy, France, the United Kingdom, Sweden, Belgium, India, and Canada. Additionally, strong U.S. leadership in physical chemistry is apparent by the 40 percent rate for U.S. contributions of papers to the *Journal of Chemical Physics*.

In journals that publish many but not exclusively physical chemistry topics, *Physical Review Letters* and *Physical Review A*, U.S. authors rep-

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resent 43 and 32 percent, respectively, of the contributions. In the more specialized but not exclusively physical chemistry journals, U.S. authors contributed 35 percent of the papers in *Langmuir* and 23 percent of the papers in *Surface Science*. It should be noted that *Surface Science* is published in Europe.

U.S. scientists were responsible for authoring 51.5 percent of highly cited physical and computational chemistry articles in 1990-1994, 47.3 percent in 1995-1999, and 49.8 percent from 2000 to 2006. Of the top hot papers, physical chemistry is the fourth most popular area of chemistry, accounting for 12.2 percent of the top hot papers from 2004 to 2006. The United States and Western Europe are responsible for most of the hot papers, contributing 50 percent and 43.8 percent, respectively. The *Journal of Physical Chemistry A and B* contained some of the most accessed ACS articles, with 65 percent (Part A) and 75 percent (Part B) of the articles coming from the United States.

The United States Is Among Leaders in Theory/Computation

Theoretical chemistry develops mathematical frameworks and formalisms to describe the chemical properties of molecular systems and their molecular interactions. Theoretical chemistry emphasizes the use of quantum and statistical mechanics to calculate the properties of molecular systems and to seek an understanding of chemical phenomena from first principles. The subarea of computational chemistry deals with the simulation of chemical processes or the calculation of chemical properties of molecules and the interaction among molecules.

To assess the current status of the U.S. contribution to theoretical chemistry, three representative subareas were examined:

Electronic structure and basic theory. Electronic structure is a branch of theoretical chemistry that develops computational methods derived from molecular quantum mechanics and applies these methods to help understand the chemical properties of molecules. Properties of molecules that electronic structure theory can determine include geometrical structures, rotational-vibrational (rovibrational) energy levels, electronic energy levels, photoelectron spectra, dipole moments, polarizabilities, and NMR spectra. Chemical properties of molecular systems not easily obtainable from existing experimental techniques can be predicted and evaluated from the application of electronic structure theory. Basic theory aims to develop new mathematical models to better describe the properties of chemical systems.

Molecular dynamics simulations provide descriptions of molecular motion in chemical systems and of the time-dependent behavior of a molecular

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system. These simulations also provide information about the structure, dynamics, and thermodynamics of large molecular systems, such as polymers, condensed phases, and biological systems.

Computer-aided chemical discovery is a rapidly growing area of theoretical chemistry that develops mathematical models of chemical processes that enable extraction and evaluation of chemical information. The goal is to test new chemical concepts to facilitate the discovery of new drugs, fuel additives, and catalysts. Discovery information that includes genetic algorithms and neural network algorithms are examples of techniques being used to evaluate how chemical systems might behave or to predict the formulation for a desired chemical property that is needed.

Assessment

The virtual congresses in theoretical/computational chemistry overall had 50 percent of the chosen speakers from the United States. While this provides evidence of U.S. leadership, the United States is not the dominant contributor.

In electronic structure and basic theory development, 47 percent of the virtual congress speakers were from the United States. A close examination of these virtual congresses showed that most of the U.S. speakers were over 50 years old, while invitees from Europe were younger. Western Europe is showing great strength, particularly in many aspects of electronic structure and basic theory development. In other areas such as Monte Carlo and molecular dynamics simulation methods, which were invented in the United States, a strong U.S. position has been maintained. The virtual congresses in the area of computer-aided discovery had 53 percent U.S. speakers and strong representation from Europe and Asia. Some organizers of the virtual congresses noted the declining U.S. leadership in electronic structure and basic theory development. One organizer attributed the decline to the fact that developing new electronic structure methods is a risky long-term investment and that the U.S. funding structure does not support this mode of operation.

U.S. authors contributed 30 percent of the papers in the leading journals that include theoretical/computational chemistry papers (*Physical Review Letters*, *Physical Review*, *Journal of Chemical Physics*, and *Journal of Physical Chemistry*). Between 2001 and 2006, there was a significant decline from 50 to 28 percent in U.S. authorship of papers in the ACS journals list.

Only eight of the 100 "hot" papers in chemistry came from theoretical/computational chemistry and only two of these came from U.S. authors. The largest numbers of hot papers in the theoretical/computational area came from Western Europe. These hot papers were split between electronic

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structure simulation and computer-aided chemical discovery. No papers from basic theory development were among the 100 hot articles.

SUMMARY

Evidence for research leadership in chemistry comes from analysis of publications, citations, highly cited papers and chemists, virtual congresses, and prizes. The strength of chemistry research across the world is very great. Overall, the United States is the leader in chemistry but does not hold a dominant position. Excellent chemists in Europe and Asia provide stiff competition for U.S. chemistry.

- In 2003 the United States published 19 percent of the world's chemistry papers. The number of papers that U.S. chemists publish has not grown and is steady at about 15,000 chemistry papers a year. The percentage of articles from non-U.S. authors in ACS journals has been increasing and is now 61 percent.
- U.S. chemists are the most prolific authors in high-profile journals such as *Science*, *Nature*, and *JACS*. U.S. chemists are also major contributors to the prestigious European journal *Angewandte Chemie*.
- U.S. chemistry leads in the total number of citations and in citations per paper. The citation rates for papers from Western Europe are 10 to 30 percent lower than for those from the United States. While U.S. chemists publish 19 percent of chemistry papers, their papers received 28 percent of the total world citations over the past 10 years.
- U.S. chemists contributed 50 percent of the 100 most cited chemistry papers. They now contribute 47 percent of the most cited papers in selected chemistry journals, down from 53 percent in 1990. Fifty percent of the world's most cited chemists are from the United States.
- U.S. chemists have been the most successful in winning international awards, including Nobel prizes.
- Virtual congress analysis supports U.S. leadership in most areas of chemistry. U.S. chemistry is particularly strong in emerging cross-disciplinary areas such as nanochemistry, biological chemistry, and materials chemistry.

Status of U.S. Leadership in Areas of Chemistry

The United States is the leader in analytical chemistry, biological chemistry, chemistry education, inorganic chemistry, and in materials chemistry and nanoscience.

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The United States is the leader or among the leaders in macromolecular chemistry, and in physical chemistry.

The United States is among the leaders in atmospheric chemistry, organic chemistry, and theoretical/computational chemistry.

The United States is among the leaders or is lagging behind the leaders in nuclear and radiochemistry.

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4

Key Factors Influencing Leadership

In this report, leadership in chemistry has been measured by such factors as the number and quality of journal articles and the composition of virtual congresses that panel members asked distinguished chemists to organize. This leadership is influenced by a multitude of factors, some of which are the result of national policy, economics, and available resources of each country in the world. The panel focused on five key factors that influence U.S. leadership in chemistry research:

- **National imperatives:** Policy decisions in response to external challenges that have influenced leadership in chemistry.
- **Innovation:** Investment and technology development mechanisms that facilitate the transition from fundamental discovery to technological applications.
- **Scientific culture:** Underlying behaviors and ways of conducting research that foster leadership in chemistry.
- **Major facilities, centers, and instrumentation:** The physical infrastructure and materiel for conducting chemistry research.
- **Human resources:** The national capacity of chemistry graduate students and degree holders.
- **Funding:** Financial support for conducting chemistry research.

NATIONAL IMPERATIVES

Challenges from other countries have always been driven by U.S. investment in research. The Soviet Union was viewed as a major challenger

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prior to its disintegration. Japan emerged as a potent competitor in the 1970s and continues to increase its prominence. Western Europe has always been a major scientific force, and the recent strengthening of science throughout the European Union has increased competition in the past decade. Most recently, there has been very strong growth of science in China and India. A recent article in *Science* reported that China is heavily funding a few strategic scientific areas, including proteomics and nanotechnology. The United States has recognized that the scientific world is becoming a flatter playing field and that this country will have to increase its efforts to remain competitive.

Industrial competitiveness relies on leadership in science. Increasingly, start-up companies exploit scientific discoveries made at universities with federal support. Technology transfer from universities to industry has been facilitated by the Bayh-Dole Act. New companies are continually being started to exploit innovations from biotechnology and nanoscience; chemists are often crucial players in these discoveries and new ventures. President Bush's "American Competitiveness Initiative" proposal, which calls for a large increase in support for research in the physical sciences and for science and math education, could have a major impact on the health of chemistry research in the United States.

National Research Council (NRC) reports on the status of chemistry have been important in setting the direction of chemistry in the United States. The 1965 Westheimer report *Chemistry: Opportunities and Needs*, the 1985 Pimentel report *Opportunities in Chemistry*, and the 2003 Breslow-Tirrell report *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering* have all highlighted opportunities in chemistry and helped explain the need for research in the chemical sciences. The 2007 NRC report *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future* explains the national imperative for investment in science.

INNOVATION

The process by which research ideas are developed and funded in the United States—our "innovation system," is another key factor influencing U.S. leadership in chemistry, improving how rapidly and easily ideas can be tested, developed, and extended. The factors that influence the process are discussed below.

A Strong U.S. Industrial Sector

Leadership in chemistry research in the United States over the years has been strongly linked with the development of the U.S. chemical industry.

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According to Landau and Arora, "The rise of the research university in science and engineering (S&E) gave a strong boost to the American chemical industry,"[1] particularly in the early part of the twentieth century. And this relationship has been a vital part of the success of the United States as a nation. Landau and Arora further point out that the U.S. chemical industry: (1) "was the first science-based, high-technology industry"; (2) "has generated technological innovations for other industries, such as automobiles, rubber, textiles . . ."; and (3) "is a U.S. success story."

At the same time, the U.S. chemical manufacturing industry is not what it used to be. Once a major net exporter, the U.S. chemical industry is now essentially a net importer (trade went negative in 2000-2001).[2] Some think that today the U.S. chemical industry is, in fact, fundamentally disadvantaged relative to the rest of the world because of its dependence on oil and natural gas for raw materials, which have become less abundant and much more costly. The cost of natural gas in the United States is now 2 to 10 times higher than anywhere else in the world. The high cost of raw materials and labor in the United States. provides an incentive for investments in new plants and even new research centers outside the United States.[3]

A Variety of Funding Opportunities

The funding of our innovation system is characterized by many options, from industry to government to private foundations. This variety of sources, with different emphases, creates a spectrum of opportunities—and the direction of research is never dictated solely by any one funding source.

Industry

U.S. industry is the largest overall supporter of chemical R&D. Between 1999 and 2003, about $20 billion a year was spent on basic chemicals, resin, synthetic rubber, fibers, and filaments, pharmaceuticals and medicines related R&D.[4] Individual companies often operate their own R&D labs, and many provide funds for academic research in targeted areas related to their areas of interest. Industrial funding for research and development in academic science and engineering (S&E) fields reached an all-time high of

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[1]R. Landau, and A. Arora, 1999, "The Dynamics of Long-Term Growth: Gaining and Losing Advantage in the Chemical Industry," in *U.S. Industry in 2000: Studies in Competitive Performance*, D.C. Mowery, ed., National Academy Press, Washington D.C., pp. 17-43.

[2]W. J. Storck, 2005, "United States: Last year was kind to the U.S. chemical industry; 2005 should provide further growth," *Chemical and Engineering News* 83(2):16-18.

[3]M. Arndt, 2005, "No Longer the Lab of the World," *Business Week*, May 2.

[4]National Science Foundation/Division of Science Resources Statistics. 2003. Survey of Industrial Research and Development.

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$2.3 billion in FY 2005.[5] Technology transfer from universities to industry has become increasingly important for the U.S. innovation system. The Bayh-Dole Act has enabled the patenting of government-funded university research and the licensing of the patents to industry. Innovative research by university faculty now increasingly leads to the formation of small start-up companies to exploit discoveries first made with the help of government funding.

Government

U.S. chemists have many options for obtaining government funding, which helps stimulate innovative research. The major sources for government funding of chemistry are the National Institutes of Health (NIH), National Science Foundation (NSF), Department of Energy (DOE), and Department of Defense (DOD). In addition, the National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration (NASA), United States Department of Agriculture (USDA), National Institutes of Standards and Technology (NIST), Environmental Protection Agency, and the new Department of Homeland Security are important sources of funding for chemists. Actual research funding levels are discussed later in this chapter.

The wide variety of sources, with different emphases, creates a spectrum of opportunities. The NSF CAREER program and the NIH Beginning Investigator programs are designed to help assistant professors at the start of their independent research careers. The peer review process that underlies research funding and the extensive networking associated with advisory boards contribute to the high quality of federally funded research.

State Initiatives

There have been a growing number of state initiatives to foster innovation and stimulate economic growth. One successful example is the Ben Franklin Technology Partners (*http://www.benfranklin.org/*), which is a statewide network in Pennsylvania that operates four regional centers located throughout the state.

Universities

Many universities are now increasing research support through centers that provide community outreach. In some cases this support comes from

[5]National Science Foundation. 2007. Industrial Funding of Academic R&D Rebounds in FY 2005 (NSF 07-311).

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multiple universities and sometimes involves partnerships with industry. One example is the University of California Discovery Grants in biotechnology to promote industry-university research partnerships. Biotechnology is one of five fields supported by Discovery Grants (i.e., biotechnology, communications and networking, digital media, electronics manufacturing and new materials, and life sciences information technology). These grants enhance the competitiveness of California businesses and the California economy by advancing innovation, R&D, and manufacturing, and by attracting new investments.

Private Foundations

Private foundation funding of U.S. chemical research also plays an important role, particularly for initiation of new projects and for helping beginning investigators achieve a rapid start in their careers. The American Chemical Society's Petroleum Research Fund has been an important source of funds both for beginning investigators and established investigators who want to expand to a new area. Private foundations, including Camille and Henry Dreyfus, John D. and Catherine T. MacArthur, David and Lucile Packard, Research Corporation, and Alfred P. Sloan, have set up special programs to help assistant professors establish innovative research programs. For those working at the interface of chemistry, biology, and medicine, support from private sources such as the American Cancer Society is important.

SCIENTIFIC CULTURE

The way in which chemistry research is carried out in the United States is influenced by underlying practices and procedures that have changed over time. Several key characteristics of the U.S. scientific culture underlie leadership in chemistry research.

Cross-Sector and International Collaborations

The movement of people and ideas among academic, industrial, government, and other laboratories is vital in the transfer of new concepts and technology. Some faculty members have industrial or government experience. They may serve as consultants to industry or participate in the formation of small start-up companies. These relationships provide researchers across sectors with a greater understanding of problems beyond their limits. Cross-sector collaborations provide a channel for the transfer of knowledge and new approaches such as those developed in academia with funding from the federal government.

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Scientific collaboration across institutional boundaries in the United States is extensive and continues to grow. According to the *Science and Engineering (S&E) Indicators 2004*, the share of articles from multiple U.S. institutions increased from 48 percent in 1988 to 62 percent in 2001. Cross-sector collaboration on papers in chemistry also grew significantly from 30 percent in 1988 to 50 percent in 2001. The overall level of collaboration is lower than for other disciplines such as, biomedical research, earth and space sciences, and physics (see Figure 4-1).

The number of internationally coauthored S&E articles has also been growing. According to Science and Engineering Indicators 2004, 23 percent of all U.S. articles had at least one non-U.S. coauthor in 2001, compared with 10 percent in 1988 (see Figure 4-2). The percentage of U.S. chemistry articles with international coauthorship increased from 10 percent in 1988 to 22 percent in 2001. The level of international collaborations on articles in chemistry is lower than in physics and the earth and space sciences, which often require large international facilities.

Strong Professional Societies

With a membership of over 159,000, the American Chemical Society is by far the most important organization for U.S. chemists. The strength of the ACS publications gives U.S. chemists a competitive advantage over their foreign colleagues. The ACS facilitates communication between members through its national, regional, and local section meetings; through publication of over 35 world-class chemistry journals; and through its 33 technical specialty divisions, which provide an intellectual home for chemists with similar interests. Symposia at national ACS meetings focus attention on emerging areas of chemistry and bring chemists together to discuss current research and important developments. There is also a plethora of regional and national societies centered on specific scientific questions or specific scientific technologies that sometimes coordinate and cofund with local ACS sections. Regional examples include the Washington Carbohydrate Discussion Group and the Delaware Valley Chromatography Discussion Group. Other professional societies that are important for promoting communication and cooperation between U.S. chemists and other scientists and engineers include the Materials Research Society, the American Institute of Chemical Engineers, the NRC Chemical Sciences Roundtable, and the Council on Chemical Research.

The Gordon Research Conferences, started as a uniquely American enterprise 75 years ago, have been important in the development of U.S. chemistry. These small conferences (100 to150 participants) now take place outside the U.S., even in China, and provide an international forum for the presentation and discussion of frontier research in specialty areas

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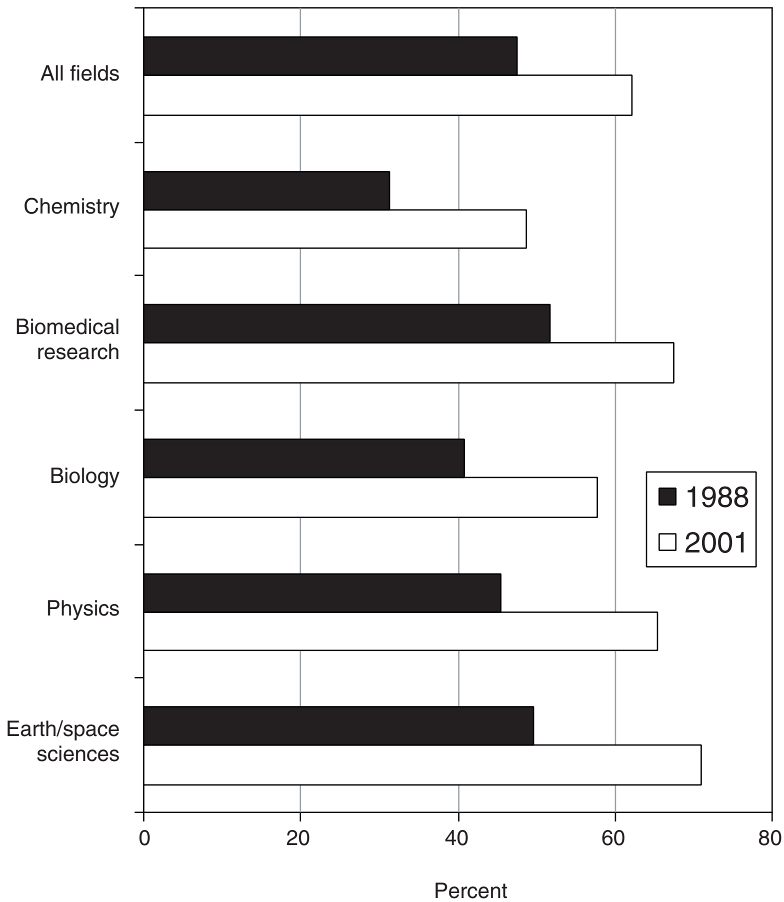

FIGURE 4-1 Extent of collaboration on U.S. S&E articles, by field, 1988 and 2001.
NOTE: Number of S&E articles with multiple institutional authors, including foreign institutions, as share of total S&E articles. Field volume is in terms of whole counts, where each collaborating institutional author is assigned an entire count.
SOURCE: National Science Foundation, *NSF Science and Engineering Indicators 2004*, Figure 5-37 (based on Appendix Tables 5-39 and 5-40).

of chemistry. The spirit of the conferences encourages open, critical, and sometimes contentious discussion of cutting edge and unpublished research. Prominent researchers and young investigators alike are challenged to support their ideas. In the process, many friendships, collegial relationships, and collaborations develop.

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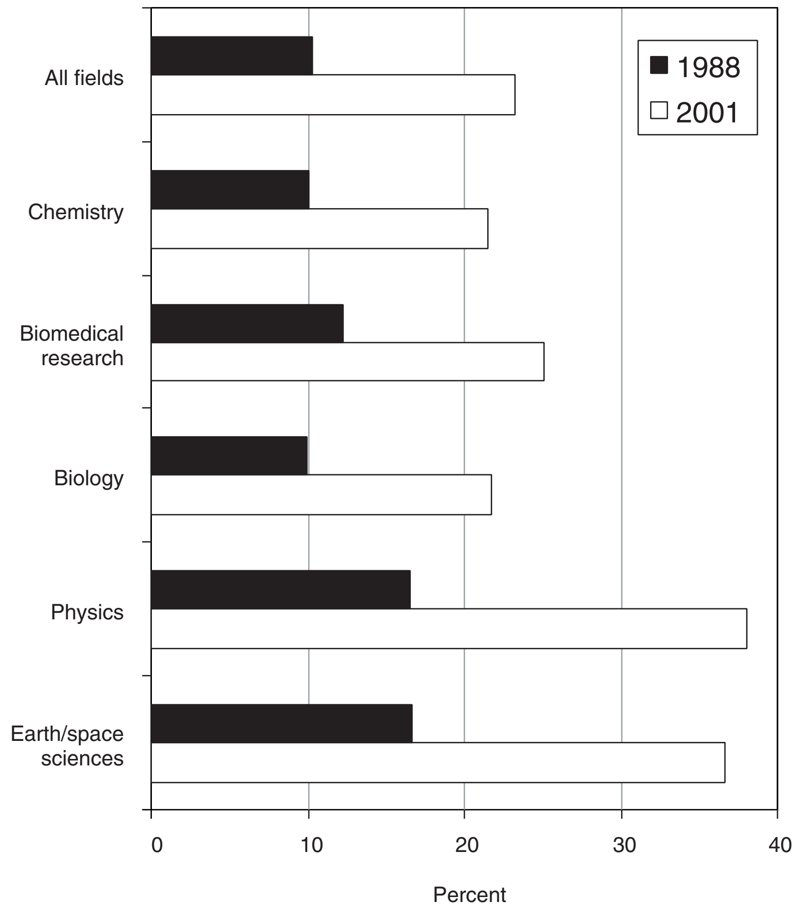

FIGURE 4-2 Extent of international collaboration on U.S. S&E articles, by field, 1988 and 2001.
NOTE: International collaboration is the number of U.S. articles with at least one non-U.S. coauthor as a share of the total number of U.S. articles. Field volume is in whole counts, where each institutional coauthor is assigned an entire count.
SOURCES: Institute for Scientific Information, Science Citation Index and Social Sciences Citation Index; CHI Research, Inc.; and National Science Foundation, Division of Science Resources Statistics, special tabulations. See Appendix Tables 5-39 and 5-40.

Fully Independent Investigators

Compared to most countries, U.S. academic chemists have longer fully independent academic careers; they start earlier and end later than chemists in Europe and Japan. U.S. academic chemists typically begin their fully

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independent careers as assistant professors in their late 20s or early 30s. This is often a highly creative period of a scientist's career, and this early independence is a strength of U.S. chemistry. At the other end of their careers, U.S. academic chemists do not face a mandatory retirement age, as their counterparts in Japan and Europe do. Consequently, senior U.S. chemists, sometimes at the height of their careers, can continue to be productive into their late 60s and beyond, while their counterparts must retire.

Mobility Across Academic Institutions

U.S. chemistry is characterized by a great deal of mobility. The typical U.S. academic chemist receives undergraduate, graduate, and postdoctoral training at three different institutions and then begins an independent career as an assistant professor at a fourth university. This movement of students and new faculty around the country rapidly spreads new ideas and modes of operation. There is less mobility in Japan and most large European countries and much less in smaller nations, where the number of research universities is limited.

CENTERS AND MAJOR FACILITIES

Excellent physical laboratory space is an important factor facilitating chemistry research, and in the U.S., laboratory space provided to chemical researchers is generally of good quality. In addition, chemistry research typically requires instrumentation, and at times, major instruments or facilities, that can only be economically provided by national facilities. In addition, because chemistry operates at the interface with many other disciplines, chemists require specialized facilities (hardware, software) used by these disciplines. Therefore, the health and competitiveness of chemistry research depend on the health and availability of cutting-edge facilities at U.S. universities and national labs. Government- and university-sponsored centers and facilities provide significant support for research activities in the United States. The Office of Basic Energy Sciences at DOE funds and operates many major facilities of relevance to chemists. Several of these are highlighted below: synchrotron radiation light sources, high-flux neutron sources, and nanoscale science research centers. There are also many NSF-funded centers and facilities, but these tend to be used more heavily at the local university level or with nearby universities. However, some of these centers do span multiple universities and provide an invaluable resource at the national level (some examples are included below). Important international facilities are included in the lists when information is available.

Some areas of chemistry often have great need for specialized facilities. For example, in macromolecular chemistry the physical characterization

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of macromolecules requires access to specialized equipment for surface analysis, rheological analysis of flow properties, thermomechanical testing, tensile strength testing, electron microscopy, and scattering techniques. National centers of excellence including national laboratories (Sandia, Los Alamos, NIST) are essential to foster this interdisciplinary research field by providing access to specialized equipment for advanced studies. Modern analytical chemistry involves both the development of new instrumentation and the clever use of commercial instrumentation. Due to high costs, state-of-the-art commercial instrumentation has become less available in training labs and research universities. Some complex instrumental systems also require teams of professional scientists for optimal operation. Access to such equipment is often best made available by establishing centers, which then require special funding mechanisms for continued operation. The types of facilities of interest to chemistry research fall into the following broad categories:

- Light sources
- Scanning probe techniques
- Nuclear magnetic resonance
- Mass spectrometry
- Cyber-enabled chemistry
- Chemical biology
- Reactors and accelerators

Light Sources

Exploring basic and applied chemistry research often requires high-energy light sources—such as synchrotron and neutron sources. These are typically available only at national facilities, both in the United States and abroad. Examples of important synchrotron sources include the Advanced Light Source (ALS), Advanced Photon Source (APS), National Synchrotron Light Source (NSLS), and Stanford Synchrotron Radiation Laboratory (SSRL) in the United States; the Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung (BESSY) in Germany and the European Synchrotron Radiation Facility (ESRF) in France; and INDUS 1/INDUS 2 in India and the National Synchrotron Radiation Research Center (NSRRC) in Taiwan.[6] Examples of important neutron sources include the Spallation Neutron Source, Oak Ridge National Laboratory, and the University of Missouri Research Reactor Center in the United States; ISIS-Rutherford-

[6]For a full list of worldwide synchrotron light sources, see *http://www.lightsources.org/cms/?pid=1000098*.

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Appleton Laboratories in the United Kingdom; and the Hi-Flux Advanced Neutron Application Reactor in Korea.[7]

Scanning Probe Techniques

Most research-intensive universities are well equipped with characterization techniques such as electron microscopy, electron and x-ray diffraction, and probe microscopy, which are used routinely to characterize small structures, small volumes, and thin films. However, the ability to characterize extremely small nanostructures or to tailor materials at an atomic level requires much more specialized equipment.

The DOE is now in the process of opening five nanotechnology centers that will provide just such capabilities. Four are described here, and a fifth will be described in connection with its biological capabilities:

The **Center for Nanoscale Materials** at Argonne National Laboratory (*http://nano.anl.gov/index.html*) will take advantage of the unique capabilities of Argonne's Advanced Photon Source. APS's hard x-rays, harnessed in a nanoprobe beamline, will provide unprecedented capabilities to characterize extremely small structures.

The **Center for Functional Nanomaterials** at Brookhaven National Laboratory (*http://www.bnl.gov/cfn/*) will provides state-of-the-art capabilities for the fabrication and study of nanoscale materials, with an emphasis on atomic-level tailoring to achieve desired properties and functions.

The **Center for Integrated Nanotechnologies** at Sandia and Los Alamos national laboratories (*http://cint.lanl.gov*) will feature low vibration for sensitive characterization, chemical/biological synthesis labs, and clean rooms for device integration. Sandia will focus on nanomaterials and microfabrication from the existing Integrated Materials Research Laboratory, while Los Alamos will focus on biosciences and nanomaterials.

The **Center for Nanophase Materials Sciences** at Oak Ridge National Laboratory (*http://www.cnms.ornl.gov/*) will concentrate on synthesis, characterization, theory/ modeling/simulation, and design of nanoscale materials. The NSF also funds several related facilities, such as the Cornell Uni-

[7]For a full list of worldwide neutron sources, see the NIST Center for Neutron Research at *http://www.ncnr.nist.gov/nsources.html*.

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versity Nanofabrication Facility,[8] which are available to external users and are part of a larger National Nanotechnology Infrastructure Network.

Nuclear Magnetic Resonance

U.S. chemistry departments typically have several moderately high field NMR spectrometers. National centers such as the NIH-funded National Magnetic Resonance Facility at the University of Wisconsin-Madison provide state of the art, very high field (800- and 900-MHz) NMR instruments not available at most institutions. The National High Magnetic Field Laboratory NMR program at Florida State University supports users pursuing research in solution and solid state NMR and in vivo magnetic resonance spectroscopy. The NMR Resource at University of California San Diego concentrates on structure determination of proteins in biological supramolecular assemblies, such as membrane proteins. The High Field Magnetic Resonance Facility at DOE's Pacific Northwest National Laboratory (PNNL)has multiple spectrometers for solid state and solution studies, including a 900-MHz NMR, a combined optical and magnetic resonance microscope, and facilities for studies of radioactive waste; about 50 non-PNNL scientists use the facility each year and access its equipment remotely by a secure Internet connection. High-field NMR is widely available to chemists around the world through local and national facilities.

Mass Spectrometry

Because use of mass spectrometry by chemists has increased greatly, most U.S. chemists have access to mass spectrometry facilities at their own institutions to confirm synthesis and support structure elucidations. Heavily used national centers provide more expensive instrumentation and more complex experiments. Most notably, a section of the National High Magnetic Field Laboratory at Florida State University provides state-of-the-art Fourier transform ion cyclotron resonance mass spectrometry. The NSF Arizona Accelerator Mass Spectrometry Laboratory is used primarily to provide radiocarbon measurements. NIH funds a number of national mass spectrometry centers to support biomedical research, including those at Boston University and the Pacific Northwest National Laboratory.

Cyber-Enabled Chemistry

NSF defines cyber-infrastructure as the distributed computer, information, and communication technologies combined with the personnel and

[8] *http://www.cnf.cornell.edu/*.

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integrating components that provide a long-term platform to empower the modern scientific research endeavor. Examples of cyber-enabled chemistry capabilities include the Pittsburgh Supercomputing Center, the Cornell Theory Center, the National Center for Supercomputing Applications in Urbana-Champaign, and the San Diego Supercomputing Center. Examples of non-U.S. supercomputing facilities used by chemists include the Barcelona Supercomputing Centers, the National Supercomputer Center in Sweden; and the high-performance computing centers in Zürich, Lausanne, and Manno Switzerland.[9] Two recently funded NSF centers are highlighted below:

Tools for Ab Initio Molecular Dynamics and Simulation Analysis This is a joint effort of researchers at the University of Illinois and Iowa State University. Their goal is to combine state-of-the-art molecular simulation techniques in a publicly available computer code, for use both by experts and nonexperts. Outcomes of this project include publicly available software tools, along with a workshop for dissemination.

Environmental Molecular Sciences Participants in this project include researchers from Pennsylvania State University. They plan to take a multidisciplinary approach to integrating information about environmental chemistry across many different scales of space and time. A database will be developed at the Center for Environmental Kinetics Analysis, an NSF-supported Environmental Molecular Science Institute, to improve communication among scientists working in various disciplines and at vastly different scales.

Chemical Biology

Chemical biology capabilities are increasingly important to chemists. A few examples of new centers providing state-of-the-art facilities and approaches are given below:

The Molecular Foundry, Lawrence Berkeley National Laboratory, (*http://foundry.lbl.gov/*) This facility provides instruments and techniques for users pursuing integration of biological components into functional nanoscale materials. It provides biological techniques in a nanotechnology environment, including molecular cloning, protein expression and purification, microbial, plant and mammalian cell culture, and preparation and characterization of cellular components and products for construction of

[9]See *http://pubs.acs.org/cen/coverstory/7918/7918supercomputer.html* and *http://www.netsci.org/Resources/Web/super.html*.

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bio/inorganic assemblies. The facility offers recombinant overexpression of proteins and nucleic acids, genetic engineering of cell lines for materials integration, and protein engineering.

Institute for Systems Biology (*http://www.systemsbiology.org/*) Building a new kind of research institute—one that can tackle the multidisciplinary challenges of systems biology requires a strategy that itself integrates many sciences, including biology, chemistry, physics, computation, mathematics, and medicine. Because the field of systems biology requires the seamless integration of these disciplines, the Institute for Systems Biology has developed a philosophy, an environment, and an administrative structure that transcend traditional organizational and disciplinary barriers. Scientists collaborate across their specialties to leverage knowledge and expertise with others at the institute and in academia and industry.

Cyberinfrastructure for Next-Generation Biomolecular Modeling The participants in this project include Teresa Head-Gordon and Martin Head-Gordon of the University of California at Berkeley, Vijay Pande of Stanford University, and Jay Ponder of Washington University. They will seek to develop and validate new ways of simulating biological molecules. They will publicly distribute the resulting software, and they will offer workshops to teach these tools to the research community at large.

Reactors and Accelerators

Nuclear reactors and particle accelerators are a critical source of radioisotopes for nuclear medicine research and practice. The need for a domestic source of radioisotopes has been documented in many reports, including most recently a Nuclear Energy Research Advisory Committee Report in 2000. Currently, there is no U.S. facility dedicated to year-round production of radioisotopes, severely compromising nuclear medicine practice and radioisotope R&D needed to advance targeted molecular therapy and other radioisotope needs for the future. Although there are large accelerators in the United States, which produce isotopes for medicine (e.g., the Brookhaven Linear Isotope Production Facility and the Isotope Production Facility at Los Alamos National Laboratory), these are part of high-energy physics accelerators, forcing medical isotope production to run only when large physics experiments are not running. Furthermore, this arrangement is subject to interruption when high-energy physics funding is interrupted. In addition, the high-flux isotope reactor at Oak Ridge, which is equipped to produce radioisotopes, now has neutron scattering experiments as a primary mission, decreasing its availability for radioisotope production

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in recent years. In contrast, France has a dedicated 70-MeV cyclotron for radioisotope production that also serves R&D and training needs.

HUMAN RESOURCES

Human resources are an essential component for leadership in chemistry. To conduct leading research, it is necessary to attract and retain the "best and brightest" S&E students from the United States and abroad as they move from undergraduate to graduate school, from graduate school to postdoctoral work, and from postdoctoral positions to faculty and research positions in academe, industry, government, and the nonprofit sector. To provide a broad context, this section first examines trends and key characteristics of S&E human resources. Then, salient features of the U.S. supply of chemists particularly at the graduate level are explored.

Strong Competition for International S&E Human Resources

In terms of sheer numbers of physical and biological sciences undergraduate degrees granted, the United States is outpaced only by India, China, and Russia (Table 4-1). However, the United States ranks lower than most industrialized nations in the percentage of its 24-year-olds who hold natural sciences and engineering degrees (see Figure 4-3). Our competitors in Europe and Asia are producing a higher percentage of S&E degree holders.

TABLE 4-1 Countries with the Largest Numbers of First University Degrees in Physical/Biological Sciences

Top 10 Countries	Number of First University Degrees (Physical/biological sciences)
India (1990)	147,036
China (2003)	103,409
Russia (1999)	101,320
United States (2002)	79,768
France (2002)	27,750
United Kingdom (2003)	27,300
Japan (2004)	19,727
Bangladesh (2002)	18,905
South Korea (2002)	12,864
Brazil (2001)	12,077

SOURCE: National Science Foundation, *Science and Engineering Indicators 2006*, Appendix Table 2-37.

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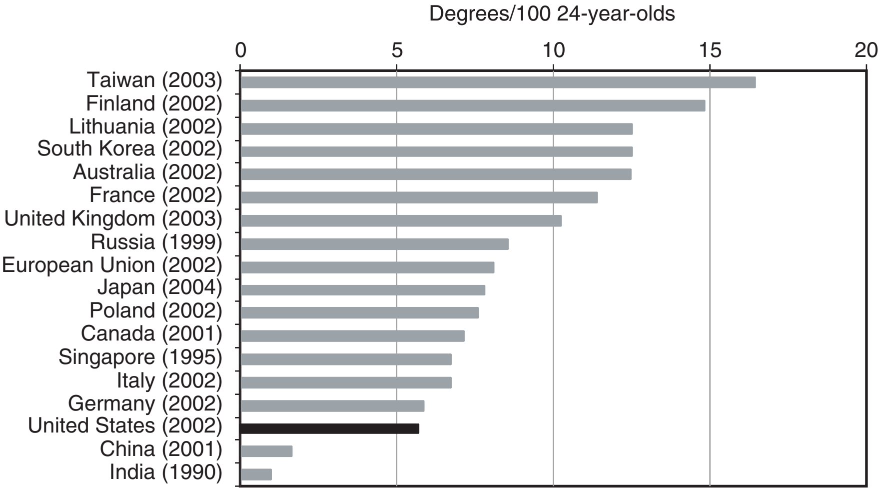

FIGURE 4-3 Natural science and engineering degrees (NS&E) per 100 24-year-olds by country/economy.
NOTE: The most recent data for India and China have likely changed significantly in recent years.
SOURCE: National Science Foundation, *Science and Engineering Indicators 2006*, based on data from Organization for Economic Cooperation and Development, Center for Education Research and Innovation, Education database, *www1.oecd.org/scripts/cde/members/edu_uoeauthenticate.asp*; United Nations Educational, Scientific, and Cultural Organization, Institute for Statistics database, *http://www.unesco.org/statistics,* and national sources.

The United States is the single largest producer of natural science and engineering doctoral degrees (see Figure 4-4). However, the number of U.S. doctorates has been declining gradually since the late 1990s, while the numbers in some countries, particularly China, are growing rapidly.

The United States increasingly relies on foreign-born scientists and engineers. In 2000, 38 percent of U.S. Ph.D. scientists and engineers were foreign-born, whereas in 1990 only 22 percent were foreign-born. Over the years the United States has been successful at attracting foreign-born scientists and engineers (see Figure 4-5), and a large portion of those who come to the United States to earn a Ph.D. in science or engineering stay here. A 2005 study found that 71 percent of foreign citizens who received S&E doctorates from U.S. universities in 2001 lived in the United States in 2003.[10] The study also found that among S&E discipline, the highest stay

[10]Finn, M. G., 2005, *Stay Rates of Foreign Doctorate Recipients from U.S. Universities, 2003*, Oak Ridge Institute for Science and Education, Oak Ridge, TN.

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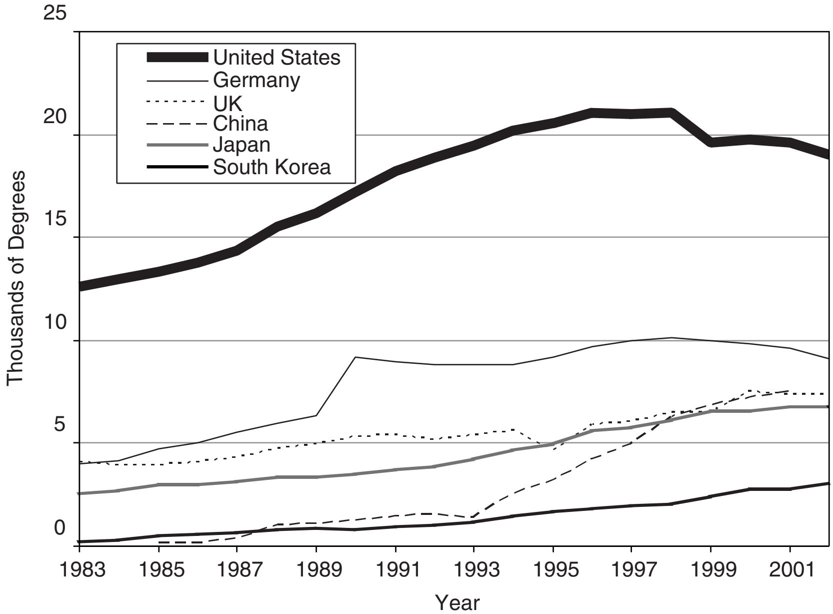

FIGURE 4-4 Natural science and engineering doctoral degrees.
SOURCE: National Science Foundation, *Science and Engineering Indicators 2006*, Figure 2-34.

rates were for computer/electrical and electronic engineering and the physical sciences. Most foreign doctorate recipients come from four countries. The stay rates for two of these countries, China (90 percent) and India (86 percent), are very high, while those for the other two, Taiwan (47 percent) and Korea (34 percent), are well below the average for all countries.

Steady Supply of Chemists in the United States

A good measure of the near-term supply of new chemists is to look at the recent trend in the numbers of graduate students in the United States, which will be discussed in more detail below. A measure of the midterm availability of U.S. research chemists is provided by the number of B.S. chemistry degrees granted in the U. S., which has drifted down by about 10 percent over the past decade. On a still longer time scale, the supply of chemists, and scientists and engineers overall, depends on the current state of the U.S. K-12 educational system. Here, there have been ongoing concerns about K-12 math and science education in the United States compared with other countries, largely based on the results of the internationally ad-

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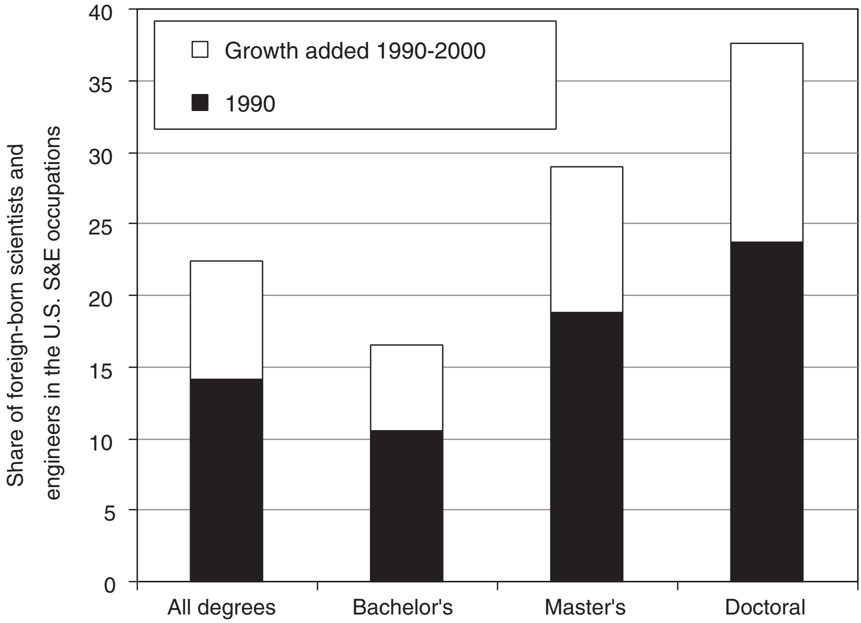

FIGURE 4-5 Share of foreign-born scientists and engineers in U.S. S&E occupations, by degree level, 1990 and 2000. NOTE: Data exclude postsecondary teachers because of U.S. Census Bureau occupation coding.
SOURCE: *Science and Engineering Indicators 2006* based on data from U.S. Census Bureau, 5-Percent Public-Use Microdata Sample, *www.census.gov/main/www/pums.html*.

ministered tests. In 2004, the NSF summarized the situation: "U.S. students are performing at or below the levels attained by students in other countries in the developed world," and "In international comparisons, U.S. student performances become increasingly weaker at higher grade levels."[11] More recent results reported by the NSF showed a more mixed picture—where U.S. fourth and eighth grade students scored above average on the international tests, but U.S. 15-year-olds scored below average.[12]

[11]National Science Foundation, *Science and Engineering Indicators 2004*, Arlington, VA (NSB 04-01) [May 2004].

[12]National Science Foundation, *Science and Engineering Indicators 2006*, Arlington, VA (NSB 06-01) [February 2006].

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Because of difficulties in locating quantitative data on chemistry human resources at the international level, the panel has concentrated on the trends in the numbers of U.S. chemistry graduate students and chemistry Ph.D. degrees. The following figures demonstrate that the number of U.S. chemistry graduate students and the number of Ph.D.s granted have remained fairly steady over the past 10 to 20 years. However, the demographics show an increasing percentage of foreign-born chemistry graduate students and new Ph.D.s.

Figure 4-6 shows that total U.S. graduate enrollment in chemistry was relatively flat between 1983 and 2004. However, examination of the residence status of graduate students shows a steady decline in the number of U.S. citizens/permanent residents enrolled in chemistry graduate programs.

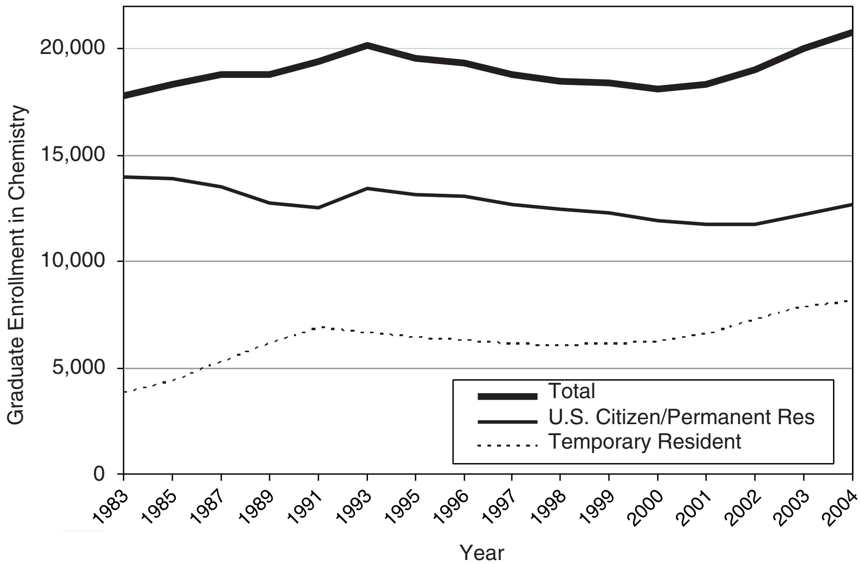

FIGURE 4-6 Total graduate enrollment in chemistry and enrollments based on residency status: U.S. citizen/permanent resident versus temporary residents, 1983-2004.
SOURCE: *Science and Engineering Indicators 2006*, Appendix Table 2-15, and National Science Foundation, Division of Science Resources Statistics, *Graduate Students and Postdoctorates in Science and Engineering: Fall 2004*, NSF 06-325, Arlington, VA.

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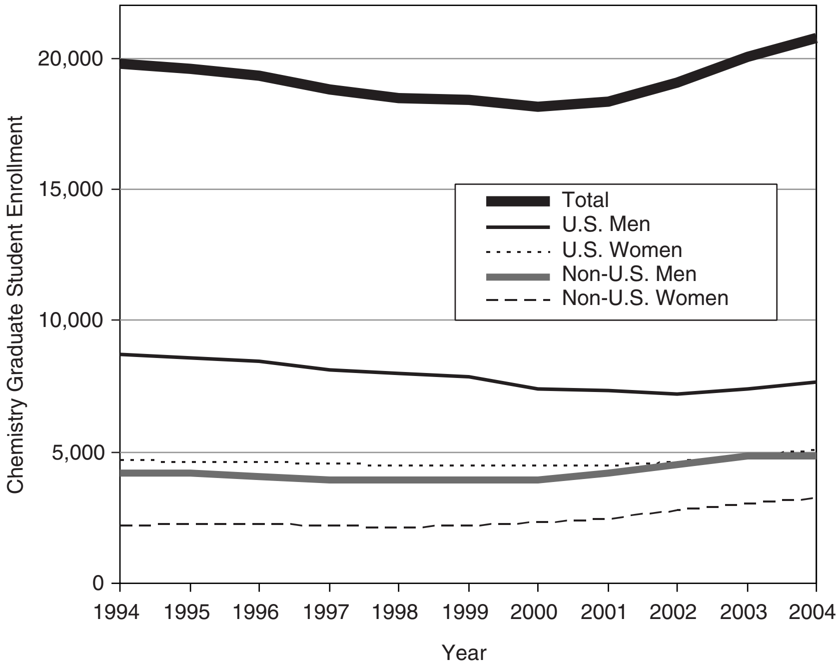

FIGURE 4-7 Total graduate enrollment in chemistry and enrollments based on residency status: U.S. citizen/permanent resident (U.S.) men and women versus temporary (non-U.S.) residents, 1994-2004.
SOURCE: National Science Foundation, National Science Foundation-National Institutes of Health Survey of Graduate Students and Postdoctorates, Resources Data System (WebCASPAR), *http://webcaspar.nsf.gov* (accessed September 25, 2006).

This decline has been largely made up by an increase in the enrollment of temporary residents.

The most recent data (2000-2004) show some growth in the number of chemistry graduate students, mainly due to an increase in non-U.S. students (see Figure 4-7).

While the numbers of black and Hispanic graduate students have grown slowly, these groups remain drastically underrepresented (see Figure 4-8).

The number of U.S. chemistry Ph.D.s granted each year reflects the health of U.S. academic chemistry and determines the availability of new researchers for the U.S. chemical industry. The number of chemistry Ph.D.s earned in the United States grew steadily between the late 1970s and early 1990s, largely due to increased numbers of doctorates awarded to tempo-

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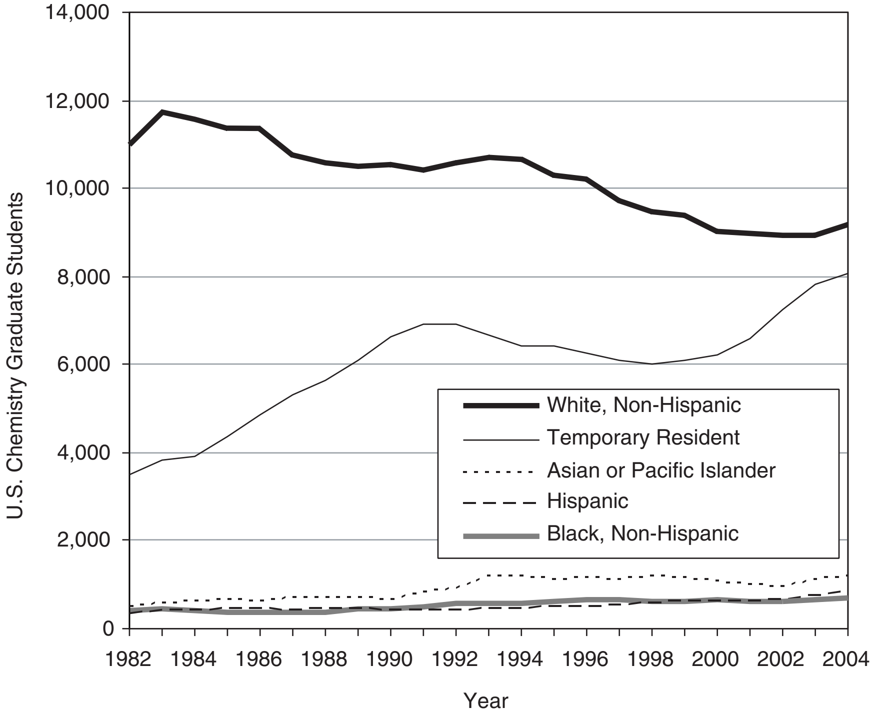

FIGURE 4-8 U.S. chemistry graduate students by race/ethnicity.
SOURCE: WebCASPAR.

rary residents and U.S. women (see Figure 4-9). Between 1994 and 2004, the number of chemistry doctorates declined slightly, especially due to declining numbers of Ph.D.s awarded to U.S. men. Over the past 15 years, the number of U.S. chemistry Ph.D.s has remained in the neighborhood of 2,000 per year, with an increasing composition earned by temporary residents.

Over the past 20 years the number of chemistry graduate students receiving support has remained largely unchanged (see Figure 4-10). Most graduate students are supported by either research or teaching assistantships.

A survey conducted by the NSF and the NIH shows that these agencies support similar numbers of graduate research assistants (RAs) and account for over 75 percent of support from federal agencies (see Figure 4-11).

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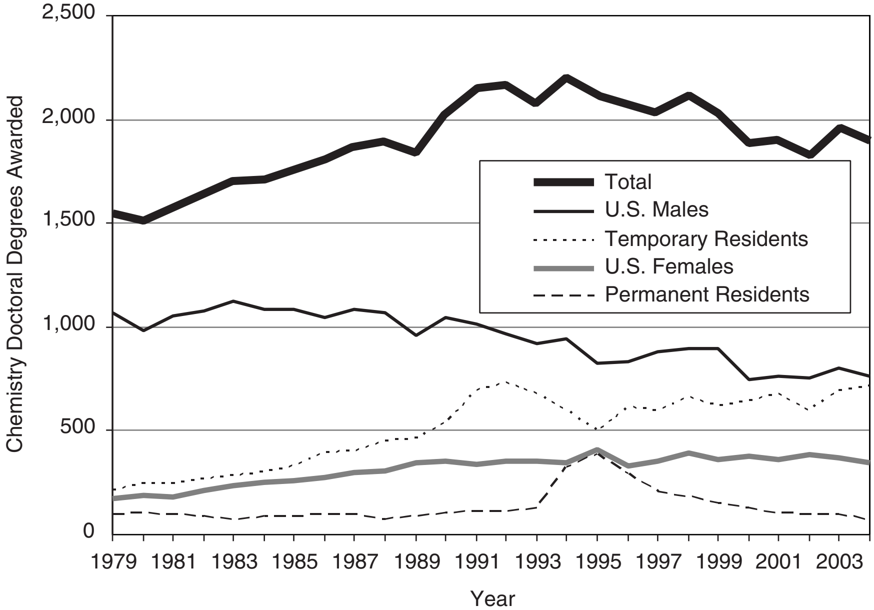

FIGURE 4-9 Earned doctoral degrees in chemistry from U.S. institutions as a function of residency status, 1979-2004.
SOURCE: National Science Foundation/Science Resource Statistics, Survey of Earned Doctorates, Integrated Science and Engineering Resources Data System (WebCASPAR), *http://webcaspar.nsf.gov* (accessed September 5, 2006).

Nonfederal sources also fund a large number of chemistry RAs and have contributed significantly to the overall growth in the number of RAs.

The number of chemistry postdoctorates has grown steadily over the years (see Figure 4-12). Three factors contributing to this increase are the rising proportion of new Ph.D.s pursuing postdoctoral work, the increasing time spent in postdoctoral positions, and the increasing number of postdoctorates recruited from Ph.D. programs abroad. The proportion of foreign-born postdoctoral researchers increased from 56 percent in 1979 to 67 percent in 2004.

Moderate Job Prospects and Salaries for U.S. Chemistry Workforce

Employment of chemistry degree holders has steadily increased over the years (see Figure 4-13). The percent change from 1999 to 2003 was

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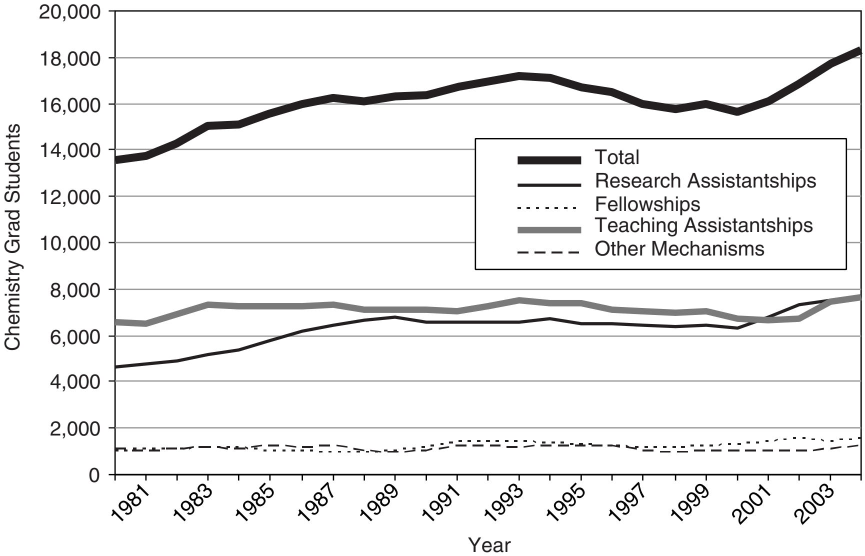

FIGURE 4-10 Full-time chemistry graduate students by mechanism of support, 1980-2004.
SOURCE: NSF/SRS, Survey of Earned Doctorates, Integrated Science and Engineering Resources Data System (WebCASPAR), *http://webcaspar.nsf.gov* (accessed September 5, 2006).

15 percent overall, 16 percent for bachelor degree holders, 19 percent for master degree holders, and 11 percent for Ph.D.s.

Chemistry employment has increased across all employment sectors (see Figure 4-14). The employment distribution has remained steady with 71 percent employed in business, 21 percent in education, and 9 percent in government.

Since a significant number of chemistry degree holders enter other occupations, the employment of chemists, as opposed to chemistry degree holders, is a slightly different story. According to the 2006 ACS annual employment survey, 3.0 percent of the survey respondents were unemployed and seeking employment (see Figure 4-15).

NSF surveys of recent chemistry Ph.D. recipients indicate some deterioration in the job market.[13] One to three years after receiving their doctorates, Ph.D. chemists reported an increase in unemployment from 0.8

[13]National Science Foundation, 2006, *Science and Engineering Indicators 2006*, Table 3-11.

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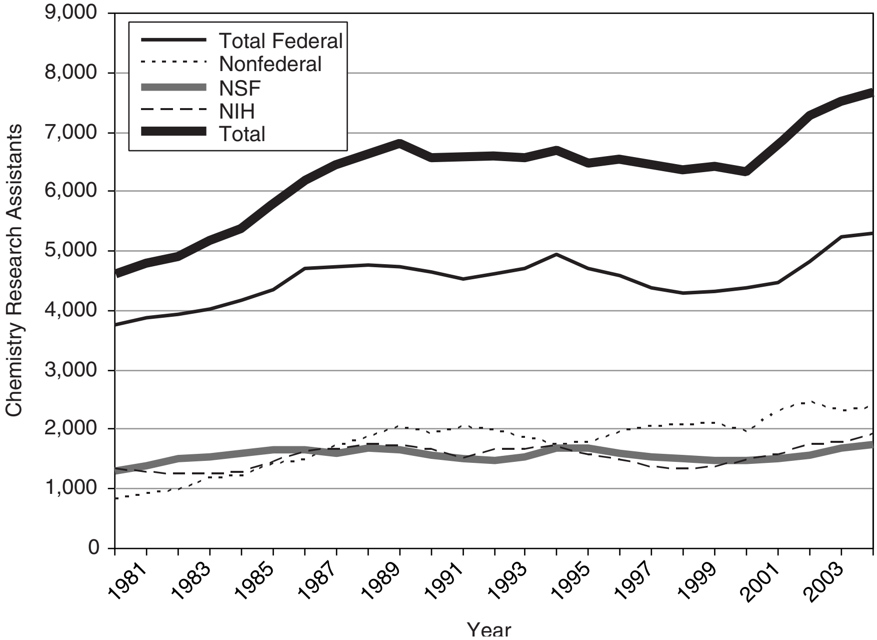

FIGURE 4-11 Full-time graduate students in chemistry on research assistantships, by funding source. (The total federal funding includes funds from the NSF, the NIH, and other federal funding sources.)
SOURCE: National Science Foundation/Science Resources Statistics, National Science Foundation-National Institutes of Health Survey of Graduate Students and Postdoctorates in S andE, Integrated Science and Engineering Resources Data System (WebCASPAR), *http://webcaspar.nsf.gov* (accessed September 5, 2006).

percent in 2001 to 2.0 percent in 2003 and an increase in involuntary out-of-field employment from 3.2 percent in 2001 to 5.6 percent in 2003.

The Bureau of Labor Statistics has commented on the job prospects for chemists over the next 5 to 10 years:

> Employment of chemists is expected to grow more slowly than the average rate (0-8 percent) for all occupations through 2014. Job growth will be concentrated in pharmaceutical and medicine manufacturing and in professional, scientific, and technical services firms. Employment in the non-pharmaceutical segments of the chemical industry, a major employer of chemists, is expected to decline over the projection period. Consequently, new chemists at all levels may experience competition for jobs in these segments, including basic chemical manufacturing and synthetic materi-

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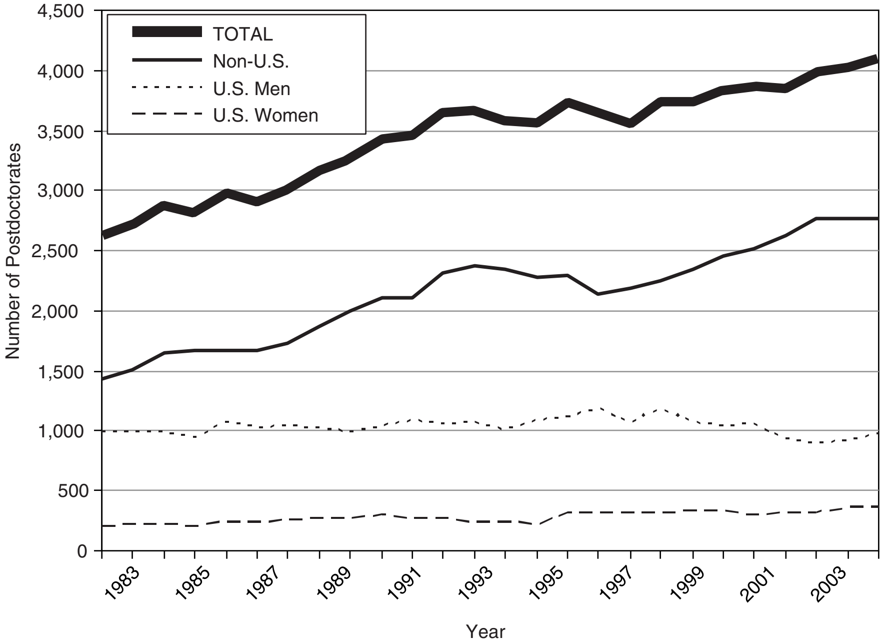

FIGURE 4-12 Numbers of chemistry postdoctorates by citizenship status and gender.
SOURCE: National Science Foundation/Science Resources Statistics, Survey of Graduate Students and Postdoctorates, Integrated Science and Engineering Resources Data System (WebCASPAR), *http://webcaspar.nsf.gov* (accessed September 25, 2006).

als. Graduates with a master's degree, and particularly those with a Ph.D., will enjoy better opportunities at larger pharmaceutical and biotechnology firms. Furthermore, those with an advanced degree will continue to fill most senior research and upper management positions, although applicants are likely to experience competition for these jobs.[14]

Data from the American Chemical Society[15] show that starting salaries for inexperienced chemists have steadily increased since 1994 (see Figure 4-16). The 3.08 percent average annual increase between 1994

[14]Bureau of Labor Statistics, 2006, Occupational Outlook Handbook, 2006-07 Edition, in *Engineers*, U.S. Department of Labor, Washington, D.C.
[15]2004 Survey on Starting Salaries of Chemists and Chemical Engineers.

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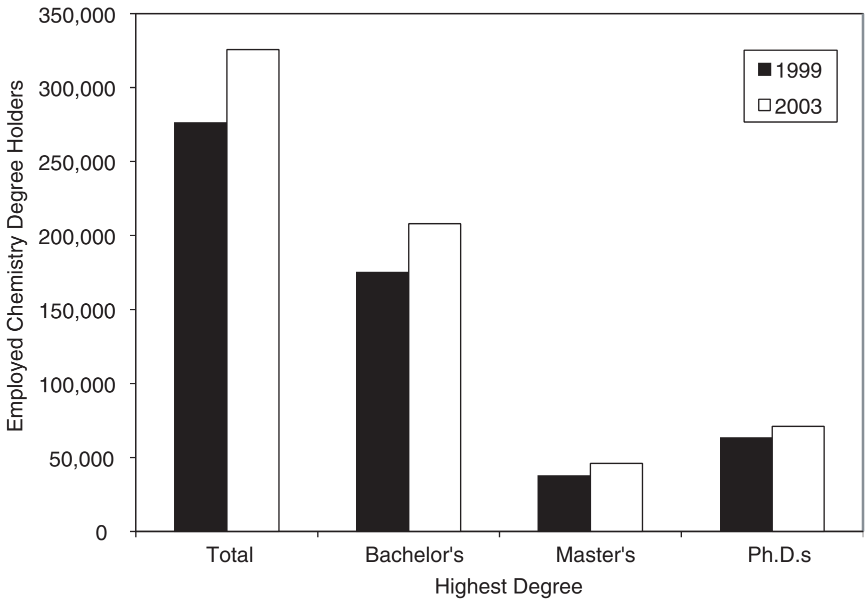

FIGURE 4-13 Comparison of employed chemistry degree holders, for 1999 and 2003.
SOURCE: Science and Engineering 2004, 2006.

and 2004 was slightly better than inflation (2.42 percent average annual increase).[16]

Earnings for more experienced chemists with Ph.D.s (see Figure 4-17) grew at an average annual rate of 3.7 percent between 1993 and 2003. This rate is 0.6 percent faster than the annual increase in starting salaries and 1.3 percent faster than inflation.[17]

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[16]The Consumer Price Index average annual increase for 1975 to 2004 was 4.42 percent (Bureau of Labor Statistics Inflation Calculator, $1 in 1975 was equivalent to $3.51 in 2004), *data.bles.gov/cgi-bin/cpicalc.pl* accessed September 8, 2006.

[17]The Consumer Price Index, average annual increase for 1993-2003 was 2.42 percent. According to the Bureau of Labor Statistics Inflation Calculator, $1 in 1993 was equivalent to $1.27 in 2003.

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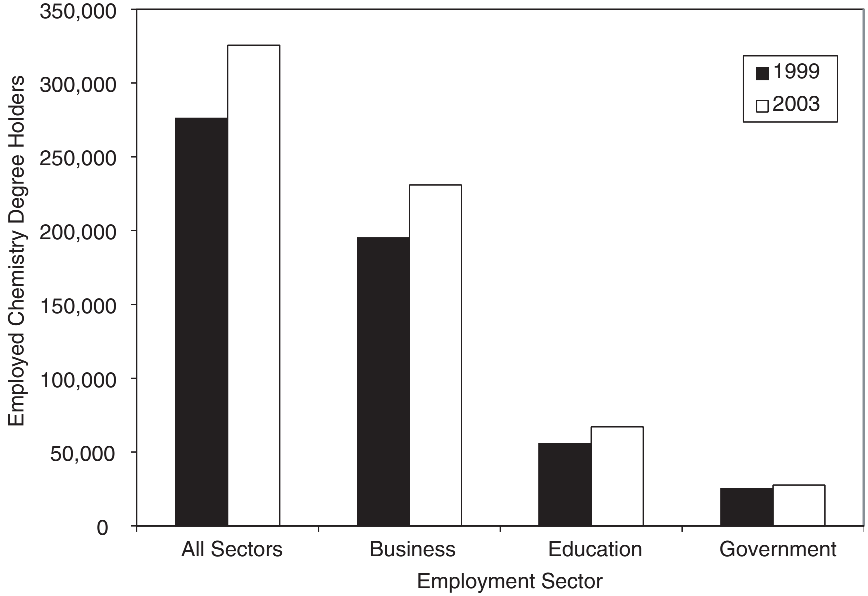

FIGURE 4-14 Comparison of employed chemistry degree holders across different sectors, 1999 and 2003.
SOURCE: Science and Engineering 2004, 2006.

R&D FUNDING

This section looks first at trends in international levels of S&E funding and then at trends in funding for chemistry in the United States.

Steady Funding for S&E in the United States

The United States spent more on science and engineering R&D between 1981 and 2002 than any other OECD country (see Figures 4-18 and 4-19). In 2003, the United States spent over $250 billion (constant 2000 U.S.$.) on total R&D; this is 43 percent of the world total. Between 1981 and 2001, the U.S. percentage of world R&D expenditures declined from 45 to 43 percent, and the G-7 percentage declined from 91 to 84 percent. The U.S. defense-related R&D expenditures were about $50 billion—an amount equivalent to Germany's total S&E expenditures.

The intensity of a nation's investment in S&E is better measured as a percentage of its gross domestic product spent on R&D. In 2003 the United

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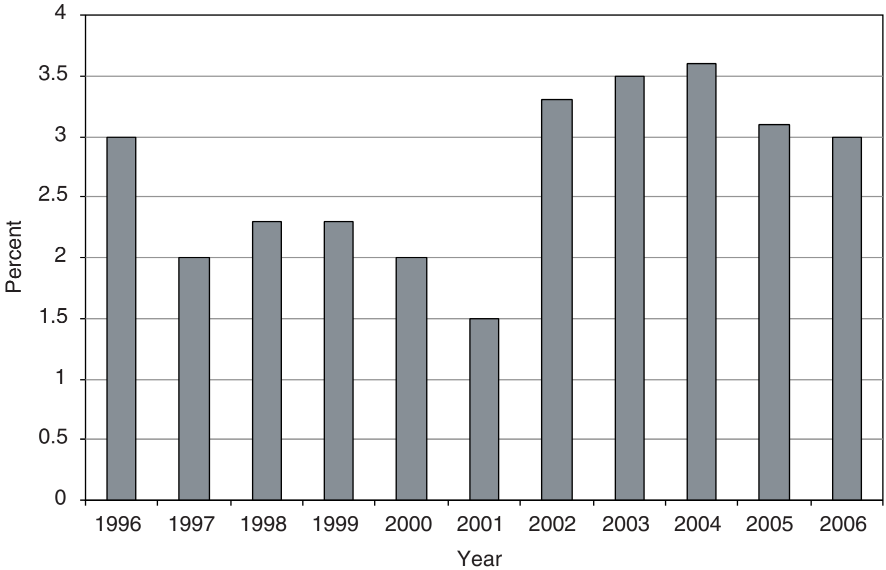

FIGURE 4-15 Unemployment rate for chemists, 1996-2006.
NOTE: As of March 1 each year. Based on population that excluded those fully retired or otherwise unemployed and not seeking employment.
SOURCE: ACS salary survey 2006, *C&E News*, 84(38), September 18, 2006.

States spent a smaller percentage of its GDP (2.2 percent) on nondefense R&D than either Japan (3.1 percent) or Germany (2.5 percent; see Figure 4-20). The European Union has a stated goal of spending 3.0 percent of GDP on research. In December 2006 the European Parliament approved the Seventh Framework Program, a 55 billion Euro, seven-year package to increase the research budget by 40 percent.[18]

Steady U.S. Funding for Chemistry R&D

In 2004 nearly $1.3 billion was spent on chemistry R&D by U.S. academic institutions (see Figure 4-21). The federal government provided 70 percent of this funding.

In terms of constant 2000 dollars, the U.S. federal obligations for total research in chemistry declined from a high of just over $1 billion in 1992

[18]M. Enserink, 2006, "European Research: Unprecedented Budget Increase Draws Faint Praise," Science 314(5805):1523-1525.

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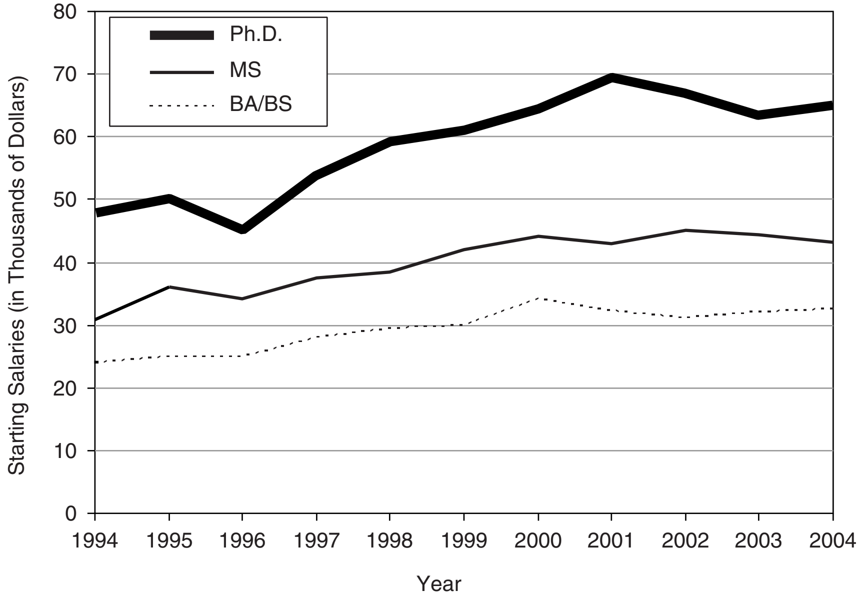

FIGURE 4-16 Median starting salaries for inexperienced chemists by degree held, 1994-2004.
SOURCE: American Chemical Society 2004 Survey on Starting Salaries of Chemists and Chemical Engineers.

to about $800 million in 1999 (see Figure 4-22). However, more recently, federal support has increased to a little more than $1 billion. Federal obligations for chemistry ranged from 3 to 4 percent of the total U.S. R&D budget between 1984 and 1998 and then dropped to 2 to 3 percent since 1999. The spike in 2000 was due to both the start of the doubling of the NIH budget and a change in the NIH accounting, which classified all of its development activities as research. The significance of the changes in the NIH budget will be discussed in the next section.

A comparison of federal funding for chemistry research with that in related areas of physical sciences and engineering is shown in Figure 4-23.

The Changing Landscape for Chemistry R&D Funding

The different federal agency contributions to the total funding for both nonacademic and academic chemistry research are shown in Figure 4-24.

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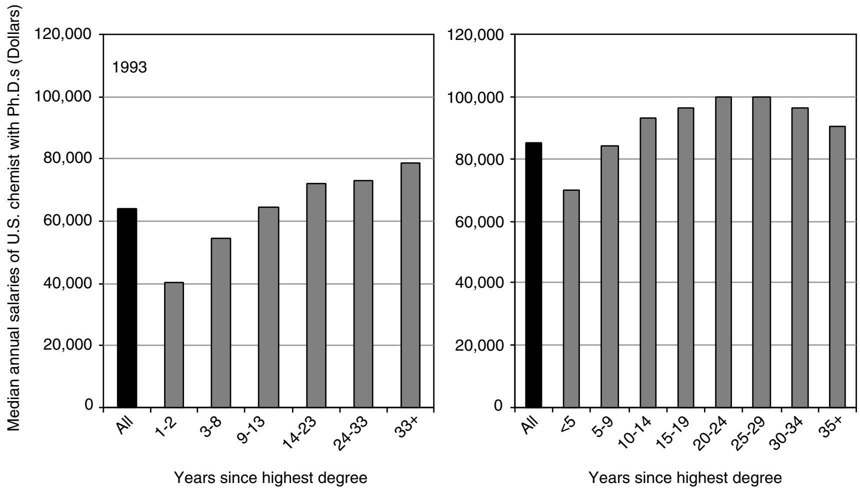

FIGURE 4-17 Median annual salaries for chemists with Ph.D.s by years since highest degree received, 1993 and 2003.
SOURCE: National Science Foundation/Science Resources Statistics, 1993 and 2003 Survey of Doctorate Recipients.

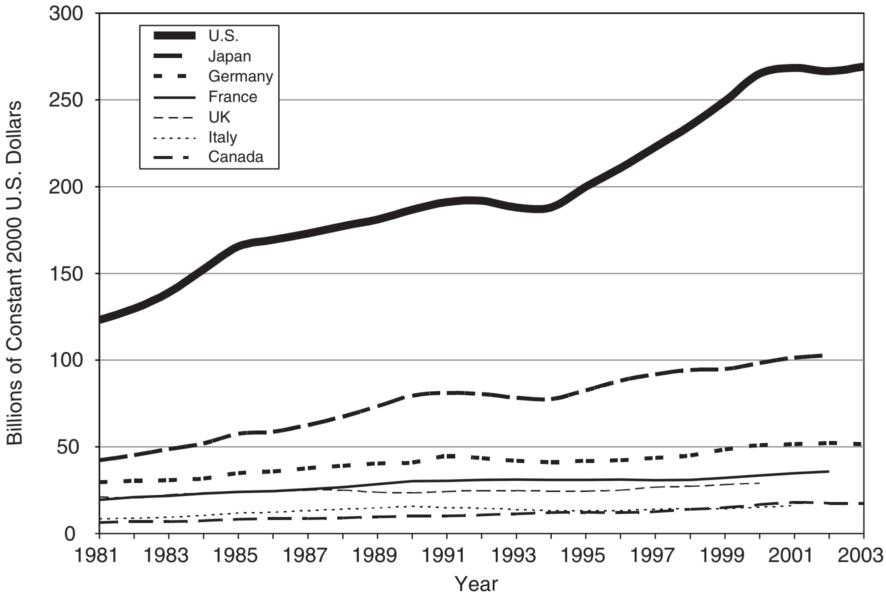

FIGURE 4-18 International R&D expenditures for select countries, 1981-2003, in billions of constant 2000 U.S. dollars.
SOURCE: *Science and Engineering Indicators 2006*, Appendix Table 4-42.

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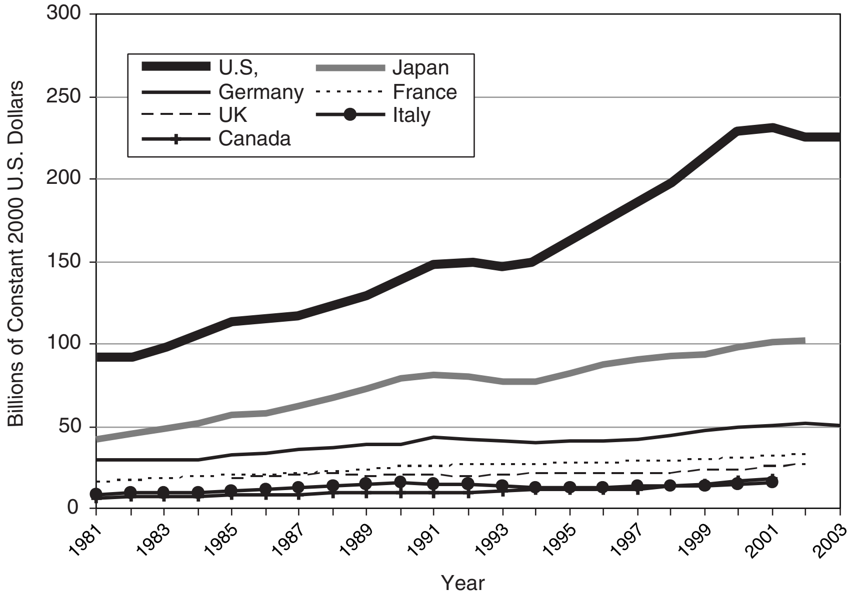

FIGURE 4-19 International nondefense R&D expenditures for select countries, 1981-2003.
SOURCE: *Science and Engineering Indicators 2006*, Appendix Table 4-43.

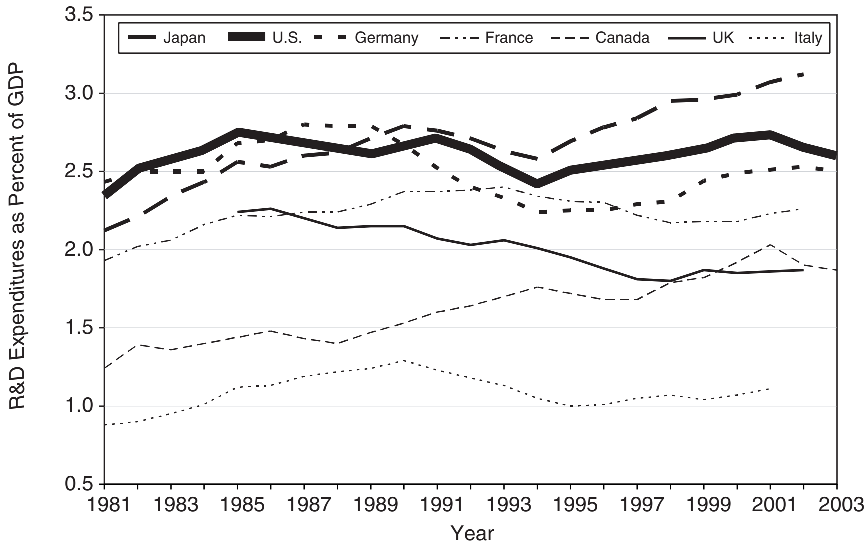

FIGURE 4-20 International nondefense R&D as percentage of GDP, by selected country, 1981-2003.
SOURCE: *Science and Engineering Indicators 2006*, Appendix Table 4-43.

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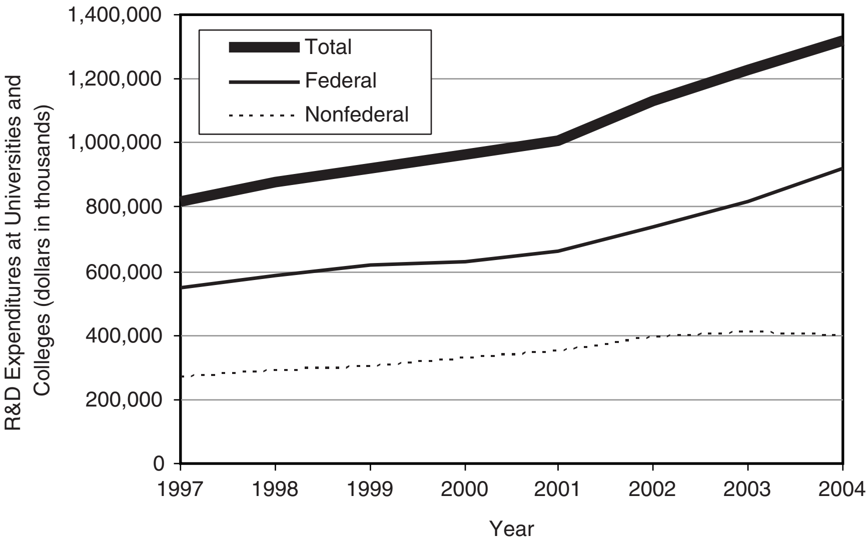

FIGURE 4-21 Federal and nonfederal R&D expenditures for chemistry at academic institutions.
SOURCE: NSF, Division of Science Resources Statistics, Survey of Research and Development Expenditures at Universities and Colleges, FY 2004.

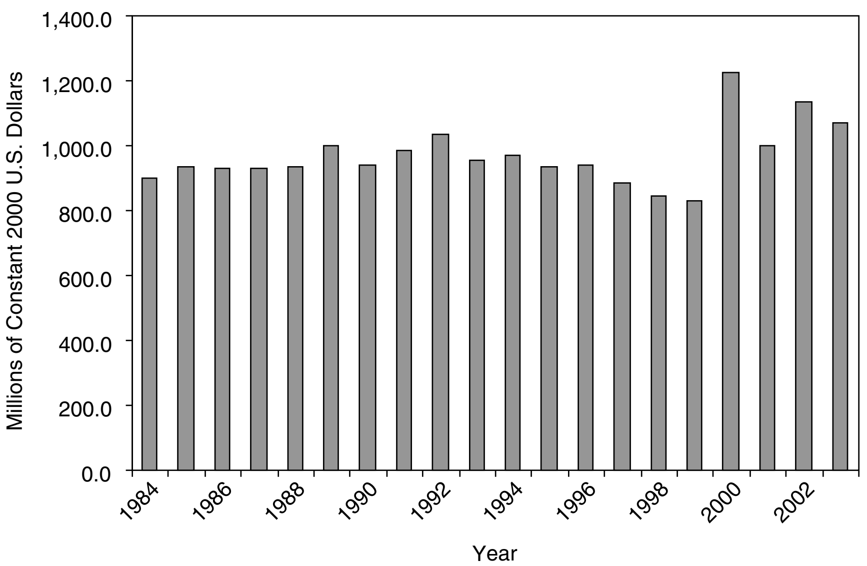

FIGURE 4-22 Federal obligations for total research in chemistry.
SOURCE: Science and Engineering Indicators 2006, Appendix Table 4-32.

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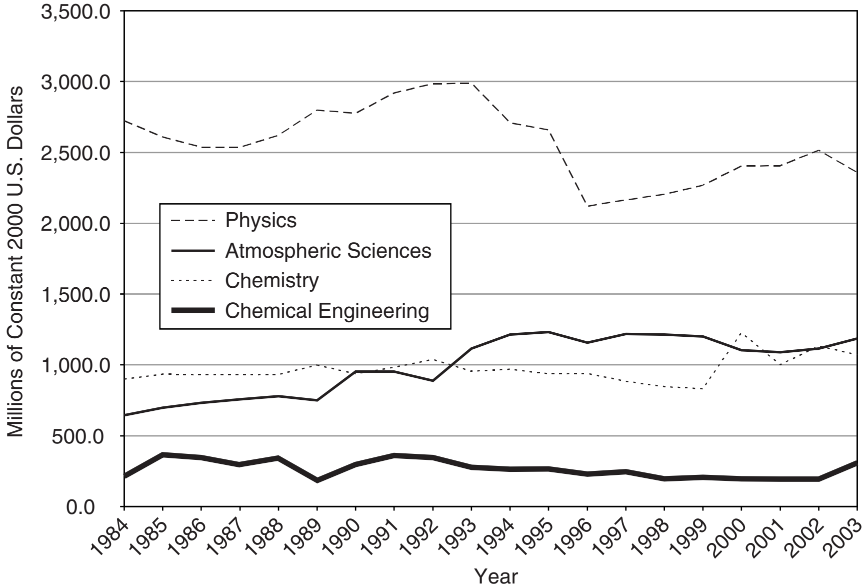

FIGURE 4-23 Federal obligations for total research, by related fields; FY 1984-2003.
SOURCE: Science and Engineering 2006, Appendix Table 4-32.

Over the years the principal sources of funding have been NSF, DOE, DOD, NIH, and, to a lesser extent, USDA. During the 1990s DOE became the largest contributor, reaching a maximum of $267 million in 1996. Starting in 2000, NIH has been the largest contributor as a result of the doubling of its budget.

DOE remains a strong contributor to chemistry research. A comparison of DOE Basic Energy Sciences funding for core research areas in chemistry, geosciences, and biosciences is shown in Figure 4-25 and that for materials is shown in Figure 4-26. Between FY 2001 and FY 2005, there were large increases for catalysis and chemical transformations ($10 million) and materials chemistry ($16 million).

As seen for total chemistry research support in Figure 4-24, support of academic chemistry research has shifted toward more reliance on NIH support (see Figure 4-27). Between 1993 and 2003, the NIH contribution to federal academic research obligations for chemistry increased from 27 to over 40 percent. The proportion of R&D funding for academic chemistry

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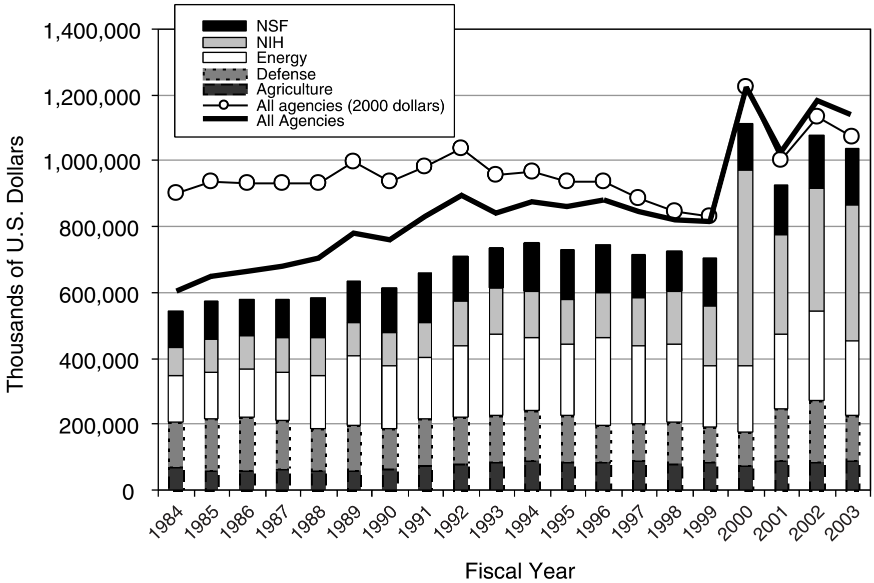

FIGURE 4-24 Federal obligations for total chemistry research, by select agency FY 1970-2003.
SOURCE: National Science Foundation, *Federal Funds for R&D*.

research coming from NSF, DOD, and USDA decreased significantly over this period.

What did the five year doubling of the NIH budget between 1998 and 2003 do for chemistry research supported by NIH? Examination of what happened at the National Institute of General Medical Sciences (NIGMS), which is a major source of chemistry support (see Figure 4-28), provides some answers. The average size of an R01 grant increased from $150,000 to $190,000 in annual direct costs. Smaller, but significant, increases also occurred in the number of NIGMS investigators with more than one NIH grant (from 33 to 42 percent) and in the total number of grants (from 820 to 991) and investigators supported (from 3,599 to 4,111). In addition, the increased funds allowed NIGMS to make some substantial investments in high-field NMR spectrometers and synchrotron radiation facilities that serve a large number of investigators. The budget increases also allowed NIGMS to initiate several larger program, including the Protein Structure Initiative.

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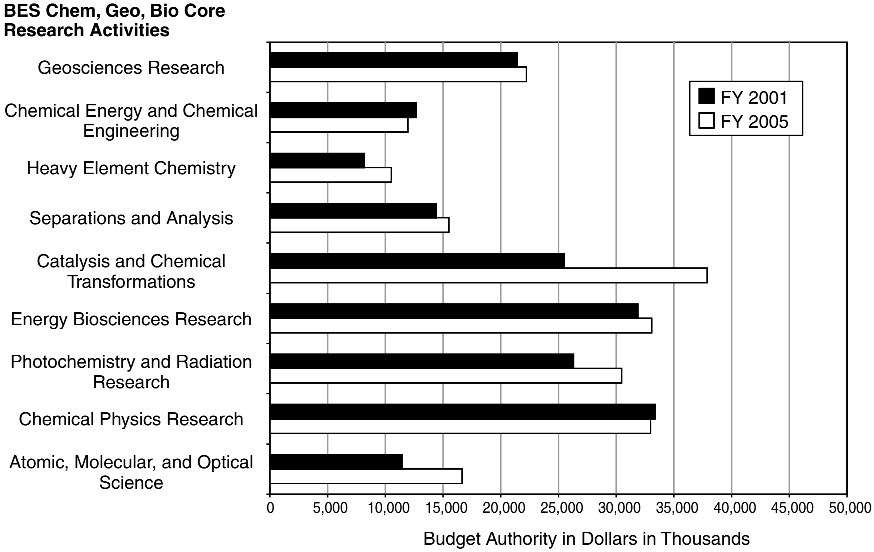

FIGURE 4-25 DOE Basic Energy Sciences funding for chemical, geological, and biological core research activities.
SOURCE: *http://www.er.doe.gov/bes/brochures/CRA.html*.

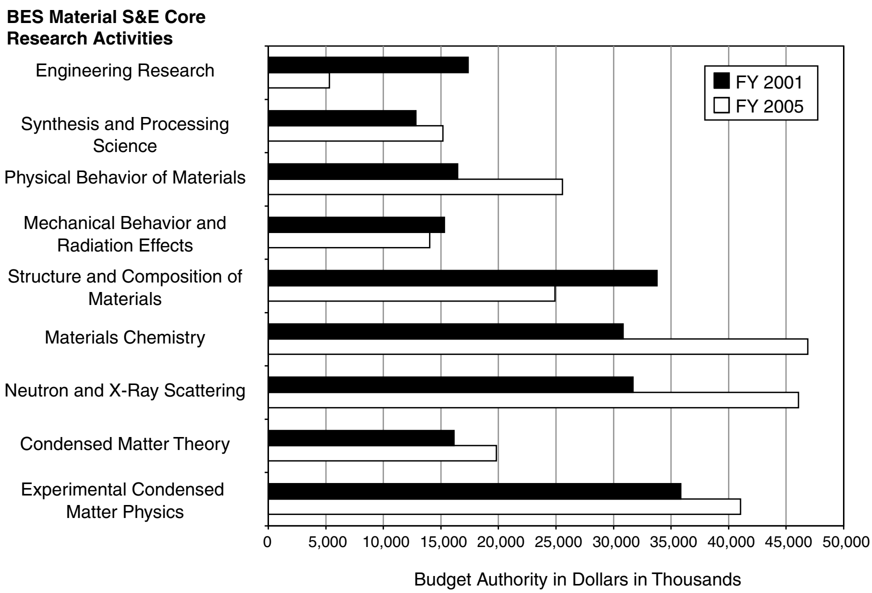

FIGURE 4-26 DOE Basic Energy Sciences funding for material science and engineering core research activities.
SOURCE: *http://www.er.doe.gov/bes/brochures/CRA.html*.

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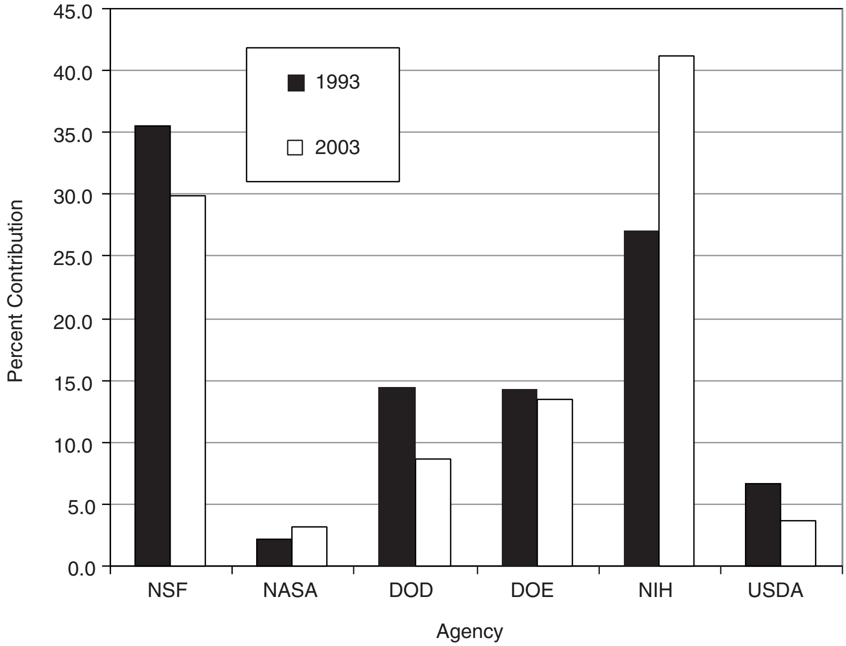

FIGURE 4-27 Federal academic research obligations for chemistry provided by major agencies.
SOURCE: *Science and Engineering Indicators 2006*, Appendix Table 5.09, and *Science and Engineering Indicators 1996*, Appendix Table 5.11.

Because NIH is the largest supporter of chemistry research, the success rate of funding for new and continuing NIH grants and the annual variability of funding rates have both a financial and a psychological impact on U.S. chemistry. The likelihood of investigator-initiated unsolicited R01 research grant applications being funded for all of NIH since 1999 is shown in Table 4-2. The success rates presented are for the original type-1 (new) and type-2 (renewal) R01 applications and do not consider resubmissions. Revision and resubmission of initially rejected type-1 application improve the likelihood of eventual funding by a factor of approximately 2, with smaller increases for rejected type-2 grants. The likelihood of funding type-1 and type-2 applications reached a low point in fiscal year 1994: approximately 12 percent for type-1 applications and 37 percent for type-2 applications. Success rates then improved and peaked between FY 1999 and 2001. Despite the doubling of the entire NIH budget between FY 1999 and FY 2003, success rates, total number of grants awarded, and total dollars committed have dropped steadily since FY 2002. In FY 2005, the decline

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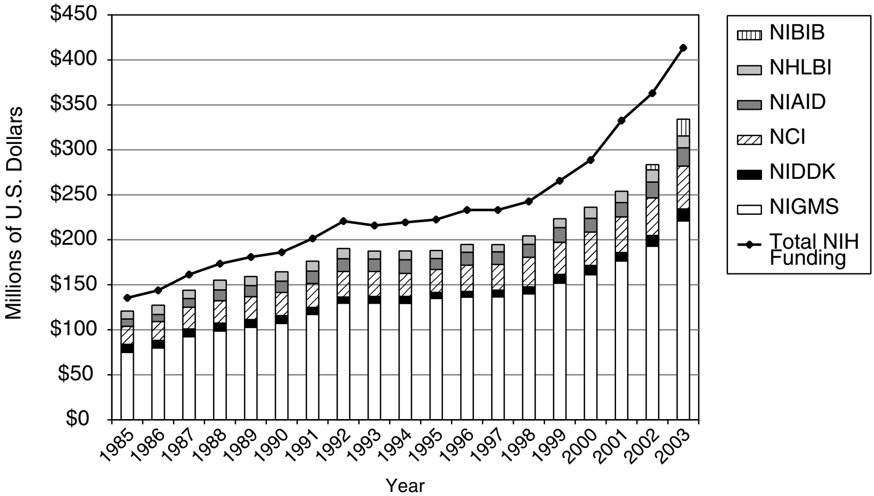

FIGURE 4-28 NIH support for chemistry department programs by institute, 1985-2003.
NOTES: NIBIB; National Institute of Biomedical Imaging and Bioengineering, NHLBI; National Heart, Lung, Blood Institute; NIAID, National Institute of Allergy and Infectious Diseases; NCI, National Cancer Institute; NIDDKD, National Institute of Diabetes and Digestive and Kidney Diseases; NIGMS, National Institute of General Medical Sciences. Chemistry department data include departments with titles such as pharmaceutical chemistry, medicinal chemistry, chemistry and chemical biology, and chemistry and biochemistry as well as departments of chemistry.
SOURCE: National Institute of General Medical Sciences Office of Program Analysis and Evaluation compilation of chemistry department support based on data from the NIH IMPAC system.

was precipitous to a success rate of 9 percent for type-1 applications and 32 percent for type-2 applications. Because the total NIH allocation for FY 2006 is less than the biomedical inflation index, a trend toward further diminished support of R01 applications is likely.

While inclusion of the success of revised applications provides a somewhat less bleak picture, each revision of a type-1 application delays the initiation of innovative research by nearly a year; the slow, uncertain revision process causes anxiety and discouragement that often lead beginning investigators to reevaluate their career choice. For an ongoing type-2 research activity, rejection casts major doubt on eventual continuation and frequently results in the breakup of teams of highly trained personnel.

The breakdown of funding for the divisions of the NSF Mathematical and Physical Sciences Directorate (MPS) is shown in Figure 4-29. The

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TABLE 4-2 Fate of Unamended (Unsolicited) NIH R01 Research Grant Applications

Fiscal Year	Number Submitted	Number Awarded	Total $ Awarded (millions)	Success Rate (%)
Type-1 grants: new submissions				
1999	8957	1761	456	19.7
2000	8626	1736	503	20.1
2001	8284	1590	501	19.2
2002	8560	1556	510	18.2
2003	9605	1477	493	15.4
2004	10624	1288	438	12.1
2005	10605	970	351	9.1
Type-2 grants: continuation (renewal) submissions				
1999	3214	1772	554	55.1
2000	3233	1708	563	52.8
2001	3100	1637	583	52.8
2002	3153	1555	559	49.3
2003	3767	1697	627	45.0
2004	3773	1530	580	40.6
2005	3896	1262	496	32.4

Declines in Funding of NIH R01 Research Grants
SOURCE: Mandel, H. G., and E. S. Vesell, 2006, ***Science*** 313(8):1387.

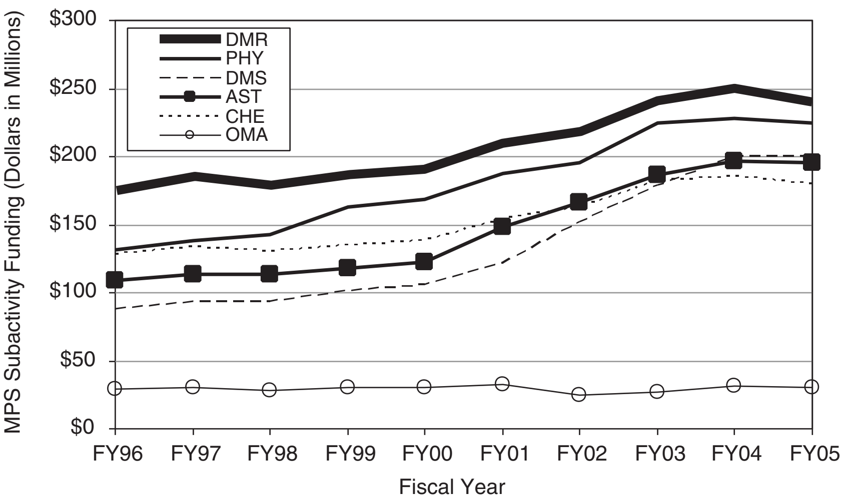

FIGURE 4-29 NSF Math and Physical Sciences Directorate funding for divisions in millions of U.S. dollars: Materials Research (DMR), Physics (PHY), Chemistry (CHE), Mathematical Sciences (DMS), Astronomical Sciences (AST), and Multidisciplinary Activities (OMA).
SOURCE: National Science Foundaton FY 2006 Budget Request, available at *http://www.nsf.gov/about/budget/* (accessed October 5, 2006).

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Chemistry Division mainly supports chemistry research at academic institutions. Changes in funding for divisions at NSF are often related to special initiatives, such as the National Nanotechnology Initiative. Funding for mathematical sciences and astronomical sciences has overtaken funding for chemistry since 2000. The large increase in funding for mathematical sciences reflects a congressionally supported initiative to make mathematical sciences a priority area over a five-year period. The increase for astronomical sciences was related in part to an MPS initiative, "Physics of the Universe," linked to an NRC report, *Connecting Quarks with the Cosmos*. The MPS budget request for 2007 (not shown in Figure 4-30) proposes an increase for the Chemistry Division related to an initiative on the molecular basis of life processes.

The research proposal funding rate for NSF's Chemistry Division is shown in Table 4-3. The funding or success rate for proposals is the total number of grant applications funded in a given fiscal year divided by the number of different grant applications that were peer reviewed. While the number of awards has remained fairly stable and the median annual size of awards increased between 1997 and 2005, the funding rate for awards has steadily decreased from 34 to 26 percent. (For similar data for CHE funding areas, see the appendix of this chapter.)

SUMMARY

U.S. research leadership in chemistry is the result of a combination of key factors, including a national instinct to respond to external challenges and to compete for leadership.

TABLE 4-3 Research Proposal Funding Rate for NSF Chemistry Division, FY 1997-2005

FY	No. of Proposals	No. of Awards	Funding Rate (%)	Median Annual Size
2005	1,635	419	26	$126,333
2004	1,708	457	27	$114,083
2003	1,520	480	32	$115,000
2002	1,407	438	31	$107,000
2001	1,343	435	32	$108,000
2000	1,241	407	33	$109,950
1999	1,124	390	35	$101,453
1998	1,267	398	31	$105,000
1997	1,378	467	34	$92,887

SOURCE: NSF Budget Internet Information System, available at *http://dellweb.bfa.nsf.gov/* (assessed October 6, 2006).

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- Over the years the United States has been a leader in innovation as a result of interactions with and support from a strong U.S. chemical industry.
- The wide range of funding sources for support of academic chemical research (including industry, multiple federal agencies, state initiatives, universities, and private foundations) facilitates innovative research.
- Key characteristics of the U.S. scientific culture that underlie current and future leadership in chemistry research include cross-sector collaborations and international partnerships, strong professional societies, early full independence of investigators, and mobility across academic institutions.
- Major centers and facilities provide key infrastructure and capabilities for conducting research and have provided the foundation for U.S. leadership. Key capabilities for chemistry research include advanced light sources, scanning probe instruments, supercomputers, very high field nuclear magnetic resonance spectrometers, advanced mass spectrometers, nuclear reactors and accelerators, and specialized facilities for chemical biology.
- There is increasingly strong competition for international S&E human resources. The United States has maintained a steady supply of Ph.D. chemistry graduates by increasingly relying on foreign-born students. Over time the number of U.S. students (particularly males) pursuing chemistry Ph.D. degrees has declined.
- Research funding for S&E overall and chemistry in particular has been steady, but an increasing percentage of support for U.S. chemical research is coming from NIH.

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APPENDIX

Research Proposal Funding Rate for NSF Chemistry Division Research Areas, FY 1997 to 2005

CHE Funding Areas	FY	Proposals	Awards	Funding Rate (%)	Median Annual Size
Analytical Separations and Measurements	2005	109	19	17	$124,333
	2004	94	23	24	$120,000
	2003	86	31	36	$100,000
	2002	74	18	24	$102,382
	2001	75	16	21	$124,880
	2000	98	24	24	$115,978
	1999	71	13	18	$122,800
	1998	103	14	14	$78,125
	1997	98	25	26	$74,750
Bimolecular Processes	2005	72	17	24	$150,000
	2004	85	21	25	$112,540
	2003	94	26	28	$132,885
	2002	86	28	33	$100,516
	2001	64	20	31	$121,260
	2000	86	26	30	$110,150
	1999	45	21	47	$117,550
	1998	44	17	39	$102,000
	1997	47	16	34	$97,414
Chemical Instrumentation	2005	134	37	28	$70,380
	2004	141	33	23	$62,041
	2003	99	28	28	$54,213
	2002	107	28	26	$60,628
	2001	93	30	32	$53,681
	2000	131	41	31	$42,375
	1999	129	44	34	$64,423
	1998	112	43	38	$121,985
	1997	255	80	31	$100,000
Chemistry Education	2005	93	4	4	$307,672
	2004	145	27	19	$38,535
	2003	8	5	63	$78,568
	2002	8	4	50	$49,938
	2001	5	4	80	$71,857
	2000	4	2	50	$66,621
	1999	3	3	100	$367,167
	1997	1	1	100	$29,954

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CHE Funding Areas	FY	Proposals	Awards	Funding Rate (%)	Median Annual Size
Electrochemistry and Surface Chemistry	2005	135	35	26	$126,667
	2004	107	29	27	$142,333
	2003	100	34	34	$122,000
	2002	117	42	36	$119,637
	2001	96	37	39	$121,333
	2000	100	27	27	$127,113
	1999	113	39	35	$108,571
	1998	94	26	28	$128,078
	1997	77	44	57	$96,724
Major Research Instrumentation	2005	121	39	32	$98,279
	2004	106	41	39	$82,581
	2003	124	46	37	$83,507
	2002	125	42	34	$84,919
	2001	138	54	39	$65,268
	2000	57	17	30	$100,000
	1999	46	18	39	$97,875
	1998	54	12	22	$88,835
Materials Synthesis and Processing	2002	78	22	28	$120,000
	2001	103	18	17	$126,385
	2000	53	15	28	$120,000
	1999	38	12	32	$103,140
	1998	39	14	36	$110,300
	1997	39	9	23	$96,250
Methodology	2005	118	27	23	$135,000
	2004	110	34	31	$124,767
	2003	111	38	34	$131,285
	2002	82	30	37	$122,217
	2001	71	29	41	$126,667
	2000	65	24	37	$117,882
	1999	41	18	44	$115,470
	1998	92	34	37	$102,980
	1997	94	35	37	$86,375
Nanoscale: Exploratory Research	2003	30	2	7	$100,000
	2002	26	4	15	$69,500
	2001	3	3	100	$95,000
Nanoscale: Intrdisciplinary Research	2005	21	1	5	$325,000
	2004	22	1	5	$325,000
	2003	29	1	3	$262,978
	2002	28	2	7	$287,779
	2001	28	2	7	$315,000

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CHE Funding Areas	FY	Proposals	Awards	Funding Rate (%)	Median Annual Size
Nanoscale: Science and Engineering Center	2001	1	1	100	$3,295,000
Physical and Inorganic	2005	143	34	24	$136,500
	2004	138	42	30	$124,833
	2003	98	35	36	$113,000
	2002	77	31	40	$120,000
	2001	50	23	46	$148,233
	2000	49	18	37	$125,000
	1999	53	20	38	$126,933
	1998	54	27	50	$130,000
	1997	57	19	33	$112,667

SOURCE: NSF Budget Internet Information System available at *http://dellweb.bfa.nsf.gov/* (assessed October 6, 2006).

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5

Likely Future Position: Increasing Challenges to U.S. Leadership in Chemistry

Earlier in this report the panel assessed the current position of U.S. research in chemistry relative to that in other regions or countries (Chapter 3) and identified the key factors influencing relative U.S. performance in chemistry (Chapter 4). In this chapter the panel addresses the third part of its charge concerning the future of U.S. chemistry: "On the basis of current trends in the United States and abroad, what will be the relative U.S. position in the near term and in the longer term?"

The short answer is that the current U.S. lead in chemistry will continue to shrink as the chemistry world becomes "flatter"[1] and more competitive. At the same time, chemistry makes many significant contributions to U.S. economic competitiveness and national quality of life; broad public benefits are now derived from past investments in chemistry. Overall, the panel believes that the science has never been more exciting nor the opportunities to gain new knowledge ever been greater than today.

U.S. LEADERSHIP IN CHEMISTRY

Assuming no major change in U.S. science policy or levels of financial support, chemistry in the United States will remain stronger than in any other single country for at least the next five years. However, there will be increasing competition, not only from our traditional competitors (Germany, Japan, and the United Kingdom) but also from additional countries in the European Union (Spain and Italy, for example) and Asian countries

[1] Friedman, T. L., *The World Is Flat*, 2005, Farrar, Straus, and Giroux.

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(Korea, Taiwan, Singapore, India, and China) that are dramatically increasing their activities in chemistry. There are many countries in which both the quantity and the quality of chemical research are increasing. As the chemistry world becomes flatter and the ability to communicate across continents increases, the number of international collaborations between U.S. chemists and chemists around the globe will increase.

Analysis of data in Chapters 3 and 4 revealed trends in U.S. chemistry that the panel believes are likely to continue in the near term (two to three years) and midterm (five to seven years). Over the past decade the number of new U.S.-trained Ph.D.s has been virtually constant, the number of papers published per year by U.S. chemists has not grown, and federal research support for chemistry has struggled to keep up with inflation. In contrast, the number of Ph.D.s trained outside the United States continues to increase. The number of papers published by non-U.S. authors in both international and American Chemical Society journals is increasing. In many areas of chemistry, other countries are making strategic investments in chemistry research. Based on flat U.S. chemistry research budgets and flat numbers of students, the panel projects that other nations and regions will soon be catching up with the United States. Projections for chemistry as a whole and for various areas and subareas of chemistry are presented below.

Will the United States Continue to Lead in Chemistry Publications?

The panel projects that the percentage of chemistry papers from U.S. authors will continue to decrease over the next several years. This will not be due to a decrease in the number of U.S. papers but to an increase in the number of papers from other countries. The quality of international chemistry is also increasing, and the panel projects that this will be reflected in increased citations per paper for non-U.S. authors and result in a decrease in the U.S. lead in citations per paper. Similarly, the fractions of the most highly accessed, most highly cited, and "hot" papers coming from non-U.S. authors are expected to increase.

Will There Be a Sustainable Supply of U.S. Chemists?

The number of chemistry Ph.D.s trained in the United States has been steady at about 2,000 per year for the past several decades. However, over this time the number of U.S.citizens receiving chemistry Ph.D.s has steadily decreased mainly due to the decline of U.S. males receiving degrees. To maintain the same number of chemistry graduate students, U.S. universities have successfully attracted increasing numbers of U.S. females and students from other countries, who often stay in the United States to pursue careers

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in chemistry. In addition, U.S. universities have attracted postdoctoral associates from other countries who often enter the U.S. workforce.

It is not clear whether the United States can continue to attract the best and brightest chemists from the United States and abroad. U.S. chemistry departments continue to attract and retain outstanding international graduate students and postdoctoral research associates because of the outstanding quality of U.S. chemistry research, faculty, and facilitie, and the availability of financial support. In addition, they are attracted to the U.S. chemistry departments as an entry to a thriving economy with a strong chemical industry. Evidence of the attractiveness of U.S. chemistry is the high percentage of foreign doctorate recipients who plan to remain in the United States for work after graduation (see Table 5.1).

Until this country is able to attract more U.S.-born students to enter chemistry, the continuation of U.S. leadership in chemistry will increasingly rest on our ability to attract the best students from abroad. In an era of globalization, and of increasing mobility of top scientific talent, it is essential to maintain the highest quality and opportunity in U.S. chemistry departments. Otherwise we will lose our best people, both U.S. and foreign born. Conversely, if the best quality and opportunity can be maintained, U.S. chemistry will be even stronger, as the United States will be able to attract and retain the best overseas people as well as the best U.S. people.

However, with changes in visa policies as a result of the attacks on 9/11 (see Figure 5.1) and global leveling in research capability, the United States may be losing ground. Following 9/11, international students and postdoctoral associates found it increasingly difficult to obtain visas to study in the United States, and many traveled instead to Europe, Japan, and Australia for their graduate work. This has had a greater impact on other disciplines than on chemistry. However, because of the growth of new opportunities for Ph.D. chemists in China, India, and elsewhere, more foreign students who obtain a U.S. Ph.D. are likely to return to careers in their native countries or to other opportunities abroad. Thus, the United States is faced with

TABLE 5.1 Percentage of Foreign Doctorate Recipients Reporting Plans to Stay in the United States After Graduation, 1994-2003

	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
Definite plans to stay	34	35	42	44	46	49	49	54	52	48
Plans to stay	62	65	67	68	67	70	71	74	73	71

SOURCE: Finn, Michael G. *Stay Rates of Foreign Doctorate Recipients from U.S. Universities, 2003*, Oak Ridge, TN: Oak Ridge Institute for Science and Education, 2005.

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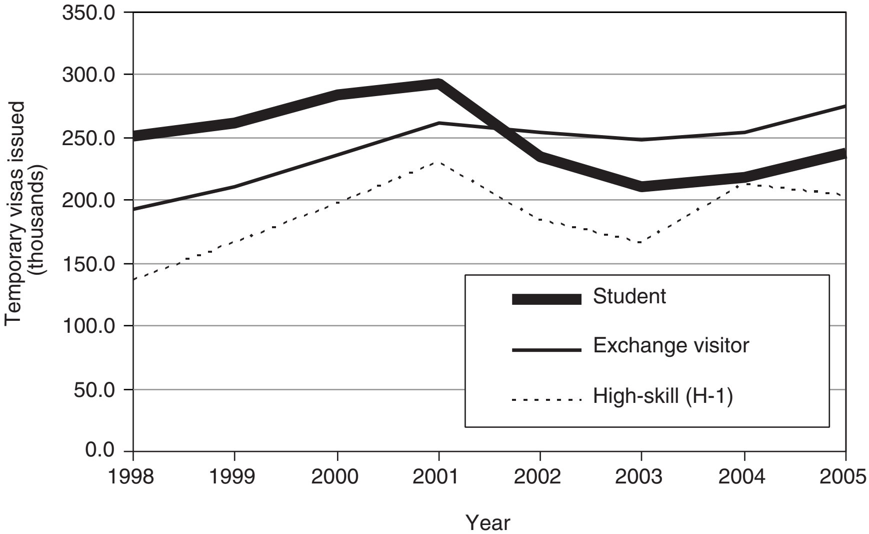

FIGURE 5.1 Student (F-1), exchange visitor (J-1), and other high-skill-(H-1) related temporary visas issued, 1998-2005.
SOURCE: National Science Foundation, *Science and Engineering Indicators 2006*.

increasing competition overall for attracting foreign graduate students and for retaining them in the U.S. workforce.

Where will the United States get the new Ph.D. chemists it needs to lead innovation in academic chemistry and the chemical industry? There has been no significant growth in the number of U.S. bachelor's degrees in chemistry over the past decade. Will the United States be able to attract more U.S. citizens into science as has been done in other countries? Will we be able to improve K-12 math and science education to help provide a longer-term source of new chemists? Will this country succeed in tapping into the pool of underrepresented U.S. minorities? While this is an important long-range goal to help solve the problem, underrepresented minorities will have limited impact on a five year timescale because so few are currently in the pipeline. Will the United States be able to continue to attract more U.S. females into chemistry careers? Currently, 31 percent of the U.S. citizen Ph.D.s in chemistry go to women. Increasing numbers of women and underrepresented minorities may help ameliorate the problem in the coming five years if foreign-born student enrollments drop significantly.

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Issues that affect the future ability of U.S. chemistry programs to attract high-quality graduate students include:

- Recruiting students from both within the United States and abroad. The decreasing numbers of U.S. citizens or permanent residents pursuing chemistry Ph.D.s is troubling.
- Improving and strengthening chemistry Ph.D. programs so that they can remain poles of attraction for young scientists.
- Retaining an open and active research environment that has been very attractive especially for non-U.S. Ph.D. students.
- Adequate financial support for students pursuing chemistry Ph.D. degrees.
- Maintaining a strong job market for chemistry graduates (especially Ph.D.s) with improved incentives and more attractive career paths.
- Increasing diversity in academia, government, and industry chemistry leadership.

What If U.S. Chemistry Research Funding Remains Flat?

Federal funding of chemistry has barely kept up with inflation over the past decade, with the notable exception of the five-year doubling of the National Institutes of Health (NIH) budget initiated in 1999. The gradual shift in U.S. funding away from individual investigator grants and toward centers will play an increasing role in identifying research foci, and this will encourage collaborations. Competition from other countries will be especially strong in areas where other countries have made strategic investments, such as nanoscience in Asia, green chemistry in Japan, biomimetic materials in Europe (Germany, the United Kingdom), proteomics in Germany and China, large-scale computation in Japan and Germany, reaction dynamics in Europe and Taiwan, and photovoltaic materials in Japan and Germany.

The panel's projection is that new funding for chemistry in the United States and around the world will be concentrated in emerging and interdisciplinary areas, which are reflected in new journals: for example, in nanoscience (*Nano Letters*), the chemistry-biology interface (*ACS Chemical Biology*, *Nature Chemical Biology*), green chemistry (*Green Chemistry* RSC), combinatorial chemistry (*Journal Combinatorial Chemistry*), and proteomics (*Journal Proteome Research*).

Many U.S. chemical companies have eliminated or significantly reduced in size their corporate or central research laboratories in order to more closely align research and development with shorter-term business opportunities. The U.S. chemical industry, which is largely global in nature, will continue to expand its applied and basic research laboratories in China and

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India rather than in the United States, Japan, and Western Europe. Technology transfer from U.S. universities to small start-up companies will likely continue. Federal funding programs for the formation of small businesses (such as the Small Business Innovation Research program) will become more critical for moving fundamental advances in chemistry to applications with societal impact.

With steady funding of research in chemistry and with expanded funding for targeted areas of chemistry, research funding for *core* areas of chemistry is decreasing. As documented in Chapter 3, several core areas of chemistry research are at serious risk and more may become at risk. Continued support of core research areas, which underlie advances in emerging areas of science, is important for the health of U.S. chemistry.

Will There Be Adequate Infrastructure to Support Basic Research?

The quality of the basic research infrastructure strongly influences the long-term health of chemistry research. The position of the U.S. research enterprise will be strongly influenced by the improvement or decline of this infrastructure, which includes organizational structure and intellectual property policies in addition to facilities and instrumentation.

The university structure in which the chemistry organization resides strongly influences the fortunes of the discipline. The high quality of academic leadership in chemistry and the excellence of the scientific research enterprise have placed chemistry departments in a position of strength at most of the top research universities in the United States. The prominence of chemistry in industry and government agencies is also well established.

Forward-looking intellectual property policies, administrative support, and access to patent expertise are improving for U.S. academic researchers in chemistry. The anticipated continuing liberalization of rules that permit academic researchers to commercialize their inventions is a positive step toward decreasing the time from invention to market. Another positive step is the growing assistance from the universities in finding industrial commercialization partners.

Chemists require excellent well-ventilated laboratories for safe research. They also require instruments for daily use and access to major frequently used instruments in their local department. Chemistry research sometimes requires major instruments or facilities that can only be economically supported by national facilities.

Major centers and facilities provide key infrastructure and capabilities for conducting research and have provided strong support for U.S. leadership in chemistry and fields depending on chemistry. Key capabilities for chemistry research include advanced light sources, scanning probe instruments, supercomputers, very high field nuclear magnetic resonance spec-

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trometers, advanced mass spectrometers, nuclear reactors and accelerators, and specialized facilities for chemical biology and nanofabrication. U.S. facilities have instrumentation that is on par with the best in the world. However, rapid advances in the design and capabilities of instrumentation can create obsolescence in five to eight years. Large central facilities must be continuously upgraded and maintained. Sustained support is essential to compete with heavy capital investments by the European Union, Japan, Korea, and China.

Federal laboratories and the national laboratories of the Department of Energy (DOE) are critical in providing unique facilities for research, and they have instrumentation that no single university could afford to put in place. An important complement is the availability of world-class scientists who engage in long-term fundamental research and provide assistance through research collaborations with the user community.

Although the United States has enjoyed a research and funding environment that has enabled the installation and operation of a diverse range of facilities to support leading-edge research in chemistry, funding for needed infrastructure seems to be in continuous jeopardy.

U.S. LEADERSHIP IN AREAS OF CHEMISTRY

U.S. chemistry now holds a leadership position in most areas of chemistry. But because of the advance of chemistry in other nations, competition is increasing and the lead of U.S. chemistry will shrink. The United States is particularly strong in emerging areas of chemical science at the interface with other disciplines. In these areas, which include nanochemistry, biological chemistry, and materials chemistry, the United States will maintain a leadership position despite growing competition, but the lead is likely to eventually erode. In some core areas where the U.S. position is not as strong, such as main group chemistry, solid state chemistry, nuclear and radiochemistry, and basic theory, U.S. leadership is likely to continue to fade. Factors that will affect the future of most areas of U.S. chemistry have been discussed already. Comments on specific concerns of the areas of chemistry dealt with in this report are given below.

The United States Will Maintain Leadership in Analytical Chemistry

The rapid commercialization and global distribution of technical advances, and the immediate global distribution of intellectual advances via commercial short courses, have the potential to level the playing field in analytical chemistry. These sales and courses are often the products of U.S. companies, which lead the world in the development and sales of analytical instrumentation. In applications areas, such as genomics, proteomics,

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chemical polymer analysis, and surface analysis, the U.S. "edge" is maintained by providing widespread and cross-disciplinary access to the most complex and expensive technology in federally funded shared resources and national laboratories. Technical innovation is being stimulated in commercial companies by the expanding global market for instruments and supplies. Technical innovation is stimulated in universities in part by the new and effective support they provide for patenting and licensing.

The United States Will Remain Among the Leaders in Atmospheric Chemistry

U.S. leadership in atmospheric chemistry will be challenged by increased competition from Europe, notably Germany and the United Kingdom. Emerging competition is also coming from China. Research in atmospheric chemistry is very interdisciplinary and distributed across three main areas: data collection in the field, laboratory simulations, and theoretical modeling. The challenge for the United States is to maintain strong efforts in each area and to facilitate efficient information exchange among the three areas.

The United States Will Maintain Leadership in Biological Chemistry

The U.S. leadership in biological chemistry is generally strong, but Asia and Europe have been heavily investing in biological chemistry. Thus, the United States is facing increasingly strong competition in chemical biology, structural biology, biocatalysis, functional genomics, and signaling pathways in living systems. While U.S. funding for biological chemistry has been strong in this area (which has tremendous implications for human health), there are some problem areas. For example, funding cuts at DOE in the basic chemistry underpinning nuclear medicine research may destabilize U.S. leadership in the area of in vivo molecular imaging. The loss of this core funding has stimulated a state-of-the-science review by a National Academies panel, which is expected to be completed in mid-2007.

The United States Will Maintain Leadership in Chemistry Education

The United States is currently the leader in chemistry education. The strength of chemistry education comes largely from the few U.S. universities where it is within the chemistry department rather than a school of education. Gains in U.S. chemistry education research will come as additional universities adopt this model and foster chemistry education research. Competition from England, Germany, and Australia is projected to increase.

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The United States Will Maintain Leadership in Inorganic Chemistry

The very strong U.S. position in bioinorganic chemistry will be maintained because of strong support from NIH and because of strong interest in this hot area of inorganic chemistry. The United States is a leader in transition metal organometallic chemistry and homogeneous catalysis, but increasing investment in this area from the European Union will increase competition. Similarly, in solid state inorganic chemistry, the moderately strong leadership position of the United States is threatened by increasing competition from Western Europe and Japan.

The U.S. weakness in main group chemistry appears to reflect both funding trends and the merger of main group chemistry with other areas so completely that it has lost its identity as a separate area. Western Europe and Japan have invested more in this area since they better appreciate the importance of main group chemistry to so many other scientific and engineering disciplines. The low U.S. research funding in this area and the small number of personnel trained in this area will continue to place the United States at a significant competitive disadvantage.

The United States Will Remain Among the Leaders in Macromolecules

The United States will continue to be a scientific leader in the synthesis and characterization of multifunctional macromolecular materials; however, university research programs will continue to refocus on rapidly emerging technology-based platforms, such as biomedical technologies, alternative energy sources, renewable resources, and electroactive devices. The United States will face increasing competition from the European Union in the areas of sustainable macromolecular chemistry and Asia-Pacific in areas dealing with electroactive macromolecular materials. While the United States has increased its attention to supramolecular chemistry, the European Union has a more directed focus on the impact of this to the emerging field on a broader range of technologies.

New faculty and incoming graduate students in macromolecular chemistry continue to show intense interest in the interface of macromolecular chemistry with emerging life sciences disciplines. In addition, many more students are now interested in entrepreneurship and working with small start-up companies.

The U.S. Leadership in Materials Chemistry and Nanoscience Will Be Challenged

U.S. leadership in materials chemistry and nanoscience is likely to decrease with time because of the high priorities given to these subfields by

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other countries. Materials chemistry and nanoscience have been an area targeted for growth in Europe. New centers for nano- and biomaterials have recently been established in Germany and the Netherlands. The field is also gaining momentum in Asia.

The United States has been successful so far in recruiting the world's best talent in materials chemistry. Recent European and Asian investments in infrastructure and research funding are likely to continue to provide increased competition. As these new, sufficiently funded, state-of-the-art centers continue to appear outside the United States, this country will face increasing difficulty in attracting leading scientists.

Materials and nanochemistry is a highly multidisciplinary field. The research in these areas will involve increasingly sophisticated fabrication and characterization facilities. There is a growing demand for specialized, capital-intensive clean rooms that can be used for "nonelectronics" applications. Collaborations will continue to become more important at the interface between materials and nanochemistry. Both international collaborations and strong partnerships between industrial and academic researchers will become more prevalent in this technology-oriented field.

The U.S. Position Among the Leaders in Nuclear and Radiochemistry Will Be Challenged

U.S. research in nuclear and radiochemistry, principally carried out at national laboratories, will continue at a leading level. The need for chemists with advanced training in nuclear and radiochemistry will likely increase in order to provide expertise in nuclear medicine and environmental fields. If the United States begins to build new nuclear reactors, there will be a severe shortage of chemists to support these facilities since very few chemists are being trained in this area. The number of U.S. universities offering graduate programs in nuclear and radiochemistry continues to decrease, as do the numbers of faculty members who can teach these subjects. The DOE has supported nuclear chemistry summer schools for undergraduates in an attempt to fill this gap in education. It is uncertain how the gap will be filled in the future, as training in nuclear and radiochemistry is declining in other countries too. If and when the United States decides that nuclear and radiochemistry programs are critical for the U.S. economy and our energy needs, additional investments will be required to attract students and faculty to meet these needs.

The United States Will Remain Among the Leaders in Organic Chemistry

The strong leadership of the United States in medicinal chemistry and drug discovery will likely continue due to strong support from NIH. In

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synthetic organic chemistry, increasing competition from Japan, Western Europe, and China will likely decrease the lead of the United States. In organometallic chemistry and homogeneous catalysis, the United States is likely to maintain its leadership. The strength of the European effort in organocatalysis is likely to grow and provide stiff competition for the United States. The erosion of support for physical organic chemistry in the United States will likely lead to a decline in U.S. leadership.

The United States Will Remain Among the Leaders in Physical Chemistry

The United States is currently among the leaders in experimental physical chemistry but is experiencing increasing competition from Western Europe and Japan. Frontier research in experimental physical chemistry that leads to the discovery of underlying principles is most often associated with the conception and development of novel instrumentation. The need to design and build unique instrumentation requires ready access to machine shop, and technical support from electronics technicians and instrument makers. Such technical infrastructure is in place and highly valued, particularly in Europe, Japan, and Taiwan, while it has been all but eliminated at most private academic institutions in the United States. The scarcity of this technical infrastructure is a major reason why the United States is among the leaders, rather than the leader, in these fields.

The U.S. Position Among Leaders in Theory/Computation Will Continue to Be Challenged

The United States is currently a leader in most areas of theoretical/computational chemistry. In basic theory, Europe has many talented young investigators. Within the next 10 years, given these demographics, the U.S. leadership will be challenged by Europe in electronic structure and basic theory development. This trend does not characterize the entire field of theoretical chemistry. For example, Monte Carlo and molecular dynamics simulation methods were invented in the United States, and to this day, the United States maintains a strong position, especially in quantum Monte Carlo calculations.

SUMMARY

On the basis of current trends in the United States and abroad, the panel projects the U.S. position in chemistry research in the near term (two to three years) and midterm (five to seven years) as outlined below:

Chemistry research in the United States will remain stronger than in

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any other single country. In the near future, U.S. chemistry will be the leader or among the world's leaders in all areas but not all subareas. Because of the advance of chemistry in other nations, competition is increasing and the lead of U.S. chemistry will shrink. There will be increasing competition from our traditional European competitors, the European Union, Japan, and other Asian countries, particularly China and India.

U.S. leadership in chemistry publications will continue to diminish. As U.S. publication rates remain steady, the number of papers from other countries is increasing. The quality of international chemistry publications also is increasing.

U.S. chemistry will be particularly strong in emerging areas. In emerging areas such as nanochemistry, biological chemistry, and materials chemistry, the United States is strong. These areas are attracting new investigators and funding initiatives. But even in these areas, the U.S. leadership position is likely to erode due to growing competition.

U.S. chemistry leadership will diminish in core areas. The growth in applications-oriented research and molecularly oriented bio- and materials-related activities has been accompanied by a parallel decrease in funding for basic research in some fundamental core areas of physical chemistry and organic chemistry. Core research areas, which underlie advances in emerging areas of science, are likely to continue to struggle for research support. Japan and Europe maintain more balanced support between core and emerging areas of chemistry. In some core subareas, such as main group chemistry, nuclear and radiochemistry, and basic theory, the U.S. position has already noticeably diminished.

The sustainability of the supply of U.S. chemists may be in jeopardy. It is likely that the number of U.S. citizens receiving chemistry Ph.D.s will continue to decrease. At the same time, U.S. chemistry may find it increasingly difficult to attract and retain outstanding international graduate students and postdoctoral research associates as chemistry in other nations improves. Continued aftershocks of the 9/11 attacks, such as increased difficulty in obtaining student visas, may continue to exacerbate the situation.

U.S. funding of chemistry research and infrastructure will remain tight. U.S. funding of chemistry is projected to continue to barely keep up with inflation. It is also likely to continue to shift away from individual investigator grants toward shorter-term goals and to be concentrated in emerging and interdisciplinary areas. Support of core research areas of chemistry, which underlie advances in emerging areas of science and in general areas

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of national priorities in healthcare, energy, and technology, will likely not be as well funded as the emerging areas. In addition, the installation and operation of a diverse range of facilities to support leading-edge research in chemistry will be equally stretched.

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APPENDIX A

Statement of Task

At the request of the Department of Energy Basic Energy Sciences Chemical Sciences, Geosciences, and Biosciences Division, and the National Science Foundation Chemistry Division, the National Academies' Board on Chemical Sciences and Technology will perform an international benchmarking exercise to determine the standing of the U.S. research enterprise relative to its international peers in the field of chemistry. The benchmarking exercise will address the following:

- What is the position of U.S. research in chemistry relative to that in other regions or countries?
- What are the key factors influencing relative U.S. performance in chemistry (i.e., human resources, equipment, infrastructure, etc.)?
- On the basis of current trends in the United States and worldwide, extrapolate to the U.S. relative position in the near and longer-term future.

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APPENDIX B

Panel Biographical Information

Chairperson

Charles P. Casey (**NAS**) is Homer B. Adkins Professor of Chemistry at the University of Wisconsin, Madison. Dr. Casey's research lies at the interface between organometallic chemistry and homogeneous catalysis, and his group studies the mechanisms of homogeneously catalyzed reactions. He received his B.S. degree from St. Louis University and his Ph.D. from the Massachusetts Institute of Technology.

Members

Joanna Aizenberg is a scientist with Bell Laboratories, Alcatel-Lucent. Her scientific interests are materials chemistry, biomineralization, biomimetics, multifunctional biomaterials, crystal engineering, nanofabrication, and control of crystal nucleation and growth. She has made seminal contributions to the understanding of the chemistry, structure, and function of biologically formed minerals and pioneered in the application of this knowledge to develop new, bio-inspired inorganic crystallization strategies. She received a Ph.D. from the Weizmann Institute of Science, Rehovot, Israel, and undergraduate and graduate degrees from Moscow State University, Moscow, USSR.

Paul S. Anderson is an internationally recognized leader in the field of drug discovery and development. During his 38-year career with Merck, Dupont-Merck, and most recently Bristol-Myers Squibb, Dr. Anderson was

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instrumental in the discovery of several of the most successful pharmaceutical products including Zocor for high cholesterol; Trusopt, for glaucoma; Aggrastat, for unstable angina; and Crixivan and Sustiva, for HIV/AIDS. Dr. Anderson obtained his B.S. in chemistry from the University of Vermont and a Ph.D. from the University of New Hampshire.

Louis E. Brus (**NAS**) is a professor of chemistry at Columbia University. He has been a pioneer in the synthesis, size control, and spectroscopy of nanometer-scale semiconductor crystallites. His elucidation of quantum-size effects in these materials is central to our understanding of the transition between molecular and bulk behavior. He received a B.S. in chemical physics from Rice University and his Ph.D. in chemical physics from Columbia University.

Sylvia T. Ceyer (**NAS**) is the J. C. Sheehan Professor of Chemistry at the Massachusetts Institute of Technology. Dr. Ceyer is a physical chemist with research interests in the area of molecule-surface reaction dynamics as related to heterogeneous catalysis, chemical vapor deposition, and plasma etching chemistry. She has uncovered sources of the apparent lack of surface reactivity under ultrahigh-vacuum conditions and then used that knowledge to effect high-pressure heterogeneous catalytic reactions in an ultrahigh-vacuum environment where microscopic reaction steps can be discerned. She received a B.A. from Hope College and a Ph.D. from the University of California, Berkeley.

Gregory R. Choppin joined the faculty at Florida State University in 1956 and from 1968 to 1976 served as chairman of the Department of Chemistry. He is a Robert O. Lawton Distinguished Professor of Chemistry at Florida State University. He received his B.S. degree in chemistry from Loyola University of the South and his Ph.D. from the University of Texas in Austin. His major research interests are inorganic and nuclear chemistry with emphasis on the lanthanide and actinide elements. Potentiometry, calorimetry, Nuclear Magnetic Resonance, and optical spectroscopy are among the methods used in his laboratory to study the thermodynamics and kinetics of complexation and redox behavior of these elements. A major focus of his laboratory is on the separation science of actinides and the environmental speciation of actinides by inorganic and organic ligands.

Catherine C. Fenselau is a professor of chemistry and biochemistry at the University of Maryland, College Park. She has been a pioneer in the application of mass spectrometry in biomedical research. Her current interests include the use of proteomic strategies to investigate cellular mechanisms of acquired drug resistance and as the basis for detection and analysis of

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microorganisms in the "detect to protect" time frame. She received her A.B. from Bryn Mawr College and her Ph.D. from Stanford University.

Joanna S. Fowler (**NAS**) is a senior chemist at the U.S. Department of Energy's Brookhaven National Laboratory. Dr. Fowler has been a major contributor to brain research and the study of diseases such as addiction, which she has investigated using the imaging technique positron emission tomography (PET). In 1976 she and her colleagues synthesized 18F-fluorodeoxyglucose, a radiotracer used in PET. Dr. Fowler earned a B.S. from the University of South Florida and a Ph.D. from the University of Colorado, Boulder.

Joseph S. Francisco is a professor of chemistry at Purdue University. His research focuses on basic studies in spectroscopy, kinetics, and photochemistry of novel transient species in the gas phase. Dr. Francisco received his B.S. from the University of Texas, Austin, and his Ph.D. from the Massachusetts Institute of Technology.

Timothy E. Long is a professor of chemistry at Virginia Polytechnic Institute and State University. His efforts are focused on the synthesis and characterization of novel macromolecules using unique combinations of step-growth and chain polymerization processes. He received a B.S. from St. Bonaventure University and a Ph.D. from Virginia Polytechnic Institute and State University.

Tobin J. Marks (**NAS**) is the Charles E. and Emma H. Morrison Professor and Vladimir N. Iptieff Professor of Chemistry at Northwestern University. Through landmark synthetic, mechanistic, and thermodynamic investigations, he and his students opened a new portion of the Periodic Table to organometallic chemistry. He has also made major advances in solid state, polymer, bioinorganic, and boron hydride chemistry and in photochemical isotope separation. He received his B.S. from the University of Maryland and his Ph.D. from Massachusetts Institute of Technology.

Michele Parrinello is chair of computational science at the Laboratory of Physical Chemistry, ETH, Zürich. Professor Parrinello's scientific interests are strongly interdisciplinary and include the study of complex chemical reactions, hydrogen-bonded systems, catalysis, and materials science. Together with Roberto Car, he introduced the abinitio molecular dynamics method, which he is still developing and applying. This method, which goes under the name of Car-Parrinello method, represents the beginning of a new field and has dramatically influenced the field of electronic structure calculations for solids, liquids, and molecules. Born in Messina, Italy,

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Dr. Parrinello obtained his Ph.D. in physics in from University of Bologna, Italy.

Chi-Huey Wong (**NAS**) is currently the President of Academia Sinica in Taiwan and Professor of Chemistry at Scripps Research Institute. Dr. Wong's principal research interests are in carbohydrate chemistry and how chemistry can be used to modify enzymes to increase or decrease enzymatic function and create better biologically active compounds. The work of his research group thus has major implications for improving human health with safer and more effective substances, such as natural products of biomedical importance. He graduated from National Taiwan University with a B.S. degree in chemistry and from the Massachusetts Institute of Technology with a Ph.D. in chemistry.

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APPENDIX C

Journal Analysis

TABLE C-1 List of Journals Examined for Publications and Citations According to Thompson ISI Essential Science Indicators Categories

	Abbreviated Jounal Name (if different from title)	2005 Impact Factor
Multidisciplinary Science		
Science		30.93
Nature		29.27
Proceedings of the National Academy of Sciences	P NATL ACAD SCI USA	10.23
Multidisciplinary Chemistry		
Angewandte Chemie International Edition	ANGEW CHEM INT EDIT	9.60
Nano Letters	NANO LETT	9.85
Journal of the American Chemical Society	J AM CHEM SOC	7.42
Chemistry-A European Journal	CHEM-EUR J	4.91
Chemical Communications	CHEM COMMUN	4.43
Chemistry Letters	CHEM LETT	1.83
Analytical Chemistry and Biochemical Research Methods		
Molecular and Cellular Proteomics	MOL CELL PROTEOMICS	9.88
Journal of Proteome Research	J PROTEOME RES	6.90
Proteomics		6.09
Analytical Chemistry	ANAL CHEM	5.64
Journal of Analytical Atomic Spectrometry	J ANAL ATOM SPECTROM	3.64
Journal of the American Society of Mass Spectrometry	J AM SOC MASS SPECTR	3.63
Electrophoresis		3.85

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TABLE C-1 Continued

	Abbreviated Jounal Name (if different from title)	2005 Impact Factor
Biochemistry and Molecular Biology		
Nature Biotechnology	NAT BIOTECHNOL	22.74
Nature Structure & Molecular Biology (*Nature Structural Biology*)	NAT STRUCT MOL BIOL	12.19
Nucleic Acids Research	NUCLEIC ACIDS RES	7.55
Journal of Biological Chemistry	J BIOL CHEM	5.85
Journal of Molecular Biology	J MOL BIOL	5.23
Journal of Nuclear Medicine	J NUCL MED	4.68
Biophysical Journal	BIOPHYS J	4.51
Proteins (Structure Function and Bioinformatics)		4.68
Glycobiology		3.51
Protein Science	PROTEIN SCI	3.62
Bioconjugate Chemistry	BIOCONJUGATE CHEM	3.94
ChemBiochem		3.94
Nuclear Medicine and Biology	NUCL MED BIOL	2.13
Carbohydrate Research	CARBOHYD RES	1.67
Environmental		
Environmental Science and Technology	ENVIRON SCI TECHNOL	4.05
Green Chemistry	GREEN CHEM	3.26
Radiochimica Acta	RADIOCHIM ACTA	0.85
Journal of Radioanalytical and Nuclear Chemistry	J RADIOANAL NUCL CH	0.46
Inorganic		
Inorganic Chemistry	INORG CHEM	3.85
Organometallics		3.47
Macromolecules		
Macromolecules		4.02
Biomacromolecules		3.62
Journal of Polymer Science Part A-Polymer Chemistry	J POLYM SCI POL CHEM	3.03
Journal of Rheology	J RHEOL	2.42
Polymer		2.85
Macromolecular Chemistry and Physics	MACROMOL CHEM PHYS	2.11
Materials Science Multidisciplinary		
Nature Materials	NAT MATER	15.94
Advanced Materials	ADV MATER	9.11
Advanced Functional Materials	ADV FUNCT MATER	6.77
Chemistry of Materials	CHEM MATER	4.82
Langmuir		3.71
Journal of Materials Chemistry	J MATER CHEM	3.69

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TABLE C-1 Continued

	Abbreviated Jounal Name (if different from title)	2005 Impact Factor
Organic and Medicinal Chemistry		
Journal of Medicinal Chemistry	J MED CHEM	4.93
Organic Letters	ORG LETT	4.37
Journal of Organic Chemistry	J ORG CHEM	3.68
Bioorganic and Medicinal Chemistry Letters	BIOORG MED CHEM LETT	2.48
Bioorganic and Medicinal Chemistry	BIOORGAN MED CHEM	2.29
Physical and Computational Chemistry		
Physical Review Letters	PHYS REV LETT	7.49
Journal of Physical Chemistry A	J PHYS CHEM A	2.90
Journal of Physical Chemistry B	J PHYS CHEM B	4.03
Journal of Chemical Physics	J CHEM PHYS	3.14
Journal of Computational Chemistry	J COMPUT CHEM	3.79
Physical Review A	PHYS REV A	3.00
Surface Science	SURF SCI	1.78

SOURCE: Thomson ISI Essentially Science Indicators.

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TABLE C-2 Analysis of Hot Papers Cited May 2004-June 2006 by area and subarea (as determined by the panel)

	No. of Articles	U.S. (%)	W. Europe (%)	Japan (%)	Asia (other) (%)	All Other (%)
ALL CHEMISTRY	147	45.3	38.4	4.7	2.9	8.7
ANALYTICAL	15	58.8	23.5	5.9	5.9	5.9
Microfluidics and miniaturization	5	16.7	50.0	16.7	0.0	16.7
Molecular/surface imaging	1	0.0	100.0	0.0	0.0	0.0
Proteomics	4	100.0	0.0	0.0	0.0	0.0
Detectors and sensors	5	83.3	0.0	0.0	16.7	0.0
Single cell analysis	1	100.0	0.0	0.0	0.0	0.0
BIOLOGICAL	15	42.1	42.1	0.0	0.0	15.8
Biocatalysis	2	25.0	50.0	0.0	0.0	25.0
Chemical/structural biology	9	27.3	54.5	0.0	0.0	18.2
In vivo molecular imaging	1	100.0	0.0	0.0	0.0	0.0
Nucleic acids and genomics	3	100.0	0.0	0.0	0.0	0.0
Signaling pathways	0	0.0	0.0	0.0	0.0	0.0
ENVIRONMENTAL	7	55.6	33.3	0.0	0.0	11.1
INORGANIC	38	40.0	42.2	2.2	2.2	13.3
Bioinorganic	3	50.0	50.0	0.0	0.0	0.0
Organometallic/ homogeneous catalysis	31	40.5	40.5	2.7	2.7	13.5
Solid state	4	25.0	50.0	0.0	0.0	25.0
Chemistry of main group elements	0	0.0	0.0	0.0	0.0	0.0
MACROMOLECULES	12	46.2	15.4	15.4	7.7	15.4
Macromolecular synthesis	4	75.0	0.0	0.0	0.0	25.0
Physical characterization and solid state structure	4	75.0	0.0	25.0	0.0	0.0
Supramolecular structure	4	0.0	40.0	20.0	20.0	20.0
Processing and rheology	0	0.0	0.0	0.0	0.0	0.0
MATERIALS/ NANOSCIENCE	54	59.7	28.4	3.0	4.5	4.5
Biomaterials	5	66.7	0.0	0.0	0.0	33.3
Nanomaterials	13	66.7	33.3	0.0	0.0	0.0
Bionano	7	75.0	0.0	0.0	12.5	12.5
Nanocrystal science/ synthesis/structure	16	48.5	39.4	6.1	6.1	0.0
Self-assembly science	5	80.0	20.0	0.0	0.0	0.0

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TABLE C-2 Continued

	No. of Articles	U.S. (%)	W. Europe (%)	Japan (%)	Asia (other) (%)	All Other (%)
ORGANIC	52	31.7	45.0	11.7	1.7	10.0
Natural products	1	0.0	0.0	0.0	0.0	100.0
Organocatalysis	24	23.1	57.7	19.2	0.0	0.0
Physical organic	8	30.0	40.0	10.0	10.0	10.0
Synthetic organic	46	35.8	45.3	11.3	0.0	7.5
Medicinal chemistry & drug discovery	0	0.0	0.0	0.0	0.0	0.0
PHYSICAL	18	50.0	43.8	0.0	0.0	6.3
Frontier in high-resolution spectroscopy	3	42.9	57.1	0.0	0.0	0.0
Frontiers in biophysical chemistry	2	50.0	50.0	0.0	0.0	0.0
Frontiers in ultrafast spectroscopy	1	100.0	0.0	0.0	0.0	0.0
Heterogeneous catalysis	5	62.5	37.5	0.0	0.0	0.0
Reaction dynamics	2	50.0	50.0	0.0	0.0	0.0
Single molecule imaging and electronics	1	50.0	50.0	0.0	0.0	0.0
Surface and interfaces	4	37.5	37.5	0.0	0.0	25.0
THEORY/COMPUTATION	11	21.4	71.4	0.0	7.1	0.0
Computer-aided chemical discovery	5	33.3	66.7	0.0	0.0	0.0
Electronic structure calculations/basic theory	6	12.5	75.0	0.0	12.5	0.0
Molecular dynamics simulations	0	0.0	0.0	0.0	0.0	0.0

SOURCE: Thompson ISI Essential Science Indicators (accessed June 22, 2006).

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APPENDIX D

Virtual World Congress

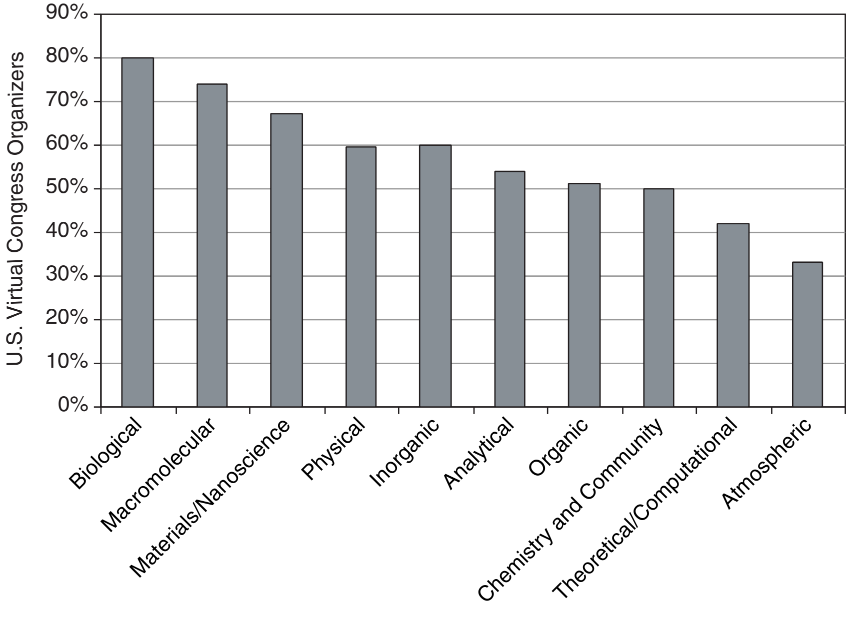

FIGURE D-1 Virtual world congress organizers by area of chemistry and U.S. residency.

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TABLE D-1 Detailed Results for Chemistry Virtual Congress

Area	Subarea	Organizers: No. of Organizers	Organizers: U.S.	Organizers: Non-U.S.	Organizers: % U.S.
Analytical	Molecular and surface imaging	6	3	3	50
	Microfluidics and Miniaturization	6	3	3	50
	Sensors and detectors	5	4	1	80
	Proteomics	6	1	5	17
	Single-cell analysis	5	4	1	80
Atmospheric Chemistry		6	2	4	33
Biological	Biocatalysis	9	5	4	56
	Chemical/structural biology	8	7	1	88
	Signaling pathways	5	4	1	80
	Nucleic acids and functional genomics	6	6	0	100
	In vivo imaging	12	10	2	83
Chemical Education		8	4	4	50
Inorganic	Chemistry of main group elements	10	6	4	60
	Homogeneous catalysis/ organometallic chemistry	7	2	5	29
	Bioinorganic/Metal coordination chemistry	10	8	2	80
	Solidstate chemistry	8	5	3	63
Macromolecular	Synthetic macromolecular chemistry	8	7	1	88
	Physical characterization and solid state structure	6	6	0	100
	Supramolecular structures	9	4	5	44
	Processing and rheology	4	3	1	75
Materials/Nanoscience	Nanomaterials: energy and Applications	7	6	1	86
	Biomaterials/bioinspired materials synthesis	10	6	4	60
	Tissue engineering/biocompatibility	9	7	2	78
	Self-assembly science	7	4	3	57
	Bionano	5	4	1	80
	Synthesis and structure/ nanocrystal and cluster science	11	6	5	55
Nuclear/radio chemistry		6	6	0	100

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Speakers				Speakers by U.S. Organizer				Speakers by Non-U.S. Organizer			
No. of Speakers	U.S.	Non-U.S.	% U.S.	No. of Speakers	U.S.	Non-U.S.	% U.S.	No. of Speakers	U.S.	Non-U.S.	% U.S.
78	49	29	63	41	31	10	76	37	18	19	49
105	66	39	63	50	36	14	72	55	30	25	55
88	61	27	69	78	57	21	73	10	4	6	40
97	46	51	47	20	10	10	50	77	36	41	47
83	64	19	77	72	55	17	76	11	9	2	82
86	52	34	60	32	24	8	75	54	28	26	52
150	73	77	49	56	38	18	68	94	35	59	37
166	124	42	75	146	117	29	80	20	7	13	35
105	72	33	69	85	64	21	75	20	8	12	40
99	82	17	83	99	82	17	83	0	0	0	0
212	133	79	63	174	115	59	66	38	18	20	47
148	72	76	49	72	42	30	58	76	30	46	39
142	54	88	38	77	35	42	45	65	19	46	29
136	66	70	49	43	30	13	70	93	36	57	39
158	116	42	73	130	96	34	74	28	20	8	71
164	94	70	57	111	61	50	55	53	33	20	62
148	94	54	64	128	89	39	70	20	5	15	25
122	83	39	68	122	83	39	68	0	0	0	0
167	65	102	39	80	38	42	48	87	27	60	31
54	27	27	50	41	22	19	54	13	8	5	62
133	99	34	74	113	89	24	79	20	10	10	50
152	95	57	63	81	55	26	68	71	40	31	56
134	109	25	81	100	83	17	83	34	26	8	76
122	77	45	63	62	48	14	77	60	29	31	48
94	73	21	78	74	56	18	76	20	17	3	85
192	125	67	65	94	71	23	76	98	54	44	55
83	43	40	52	83	43	40	52	0	0	0	0

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TABLE D-1 Continued

Area	Subarea	Organizers			
		No. of Organizers	U.S.	Non-U.S.	% U.S.
Organic	Synthetic organic chemistry	8	3	5	38
	Natural products chemistry	9	7	2	78
	Physical organic chemistry	8	4	4	50
	Organocatalysis	7	2	5	29
	Medicinal chemistry and drug discovery	9	5	4	56
Physical	Reaction dynamics	25	12	13	48
	Frontiers in high-resolution spectroscopy	19	10	9	53
	Frontier in ultrafast spectroscopy	12	9	3	75
	Frontiers in biophysical chemistry	10	7	3	70
	Frontiers in heterogeneous catalysis (fundamental and applied)	18	10	8	56
	Single-molecule imaging and electronics	6	5	1	83
	Surfaces and interfaces	19	12	7	63
Theoretical/ Computational	Electronic structure calculations/ basic theory	6	2	4	33
	Molecular dynamics simulations	9	4	5	44
	Computer-aided chemical discovery	5	3	2	60

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Speakers				Speakers by U.S. Organizer				Speakers by Non-U.S. Organizer			
No. of Speakers	U.S.	Non-U.S.	% U.S.	No. of Speakers	U.S.	Non-U.S.	% U.S.	No. of Speakers	U.S.	Non-U.S.	% U.S.
155	91	64	59	54	36	18	67	101	55	46	54
180	106	74	59	143	88	55	62	37	18	19	49
139	83	56	60	79	58	21	73	60	25	35	42
112	57	55	51	34	19	15	56	78	38	40	49
149	103	46	69	85	69	16	81	64	34	30	53
464	263	201	57	235	151	84	64	229	112	117	49
355	201	154	57	210	130	80	62	145	71	74	49
203	115	88	57	161	100	61	62	42	15	27	36
174	119	55	68	124	96	28	77	50	23	27	46
301	130	171	43	172	99	73	58	117	28	89	24
118	78	40	66	98	64	34	65	20	14	6	70
350	209	141	60	221	146	75	66	129	63	66	49
120	56	64	47	47	22	25	47	73	34	39	47
187	98	89	52	87	46	41	53	100	52	48	52
87	46	41	53	55	34	21	62	32	12	20	38

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TABLE D-2 List of Experts Who Organized the Virtual World Congress by Nominating Its Keynote Speakers

Name	Affiliation
Abbatt, Jonathan	University of Toronto, Canada
Abe, Manabu	Osaka University, Japan
Abou-Gharbia, Magid	Wyeth Pharmaceuticals
Addadi, Lia	Weizmann Institute of Science, Israel
Alario-Franco, Miguel	Complutense University of Madrid, Spain
Alivisatos, Paul	University of California, Berkeley
Allen, Heather C.	Ohio State University
Antonietti, Markus	Max Planck Institute of Colloids and Interfaces, Germany
Aono, Masakazu	RIKEN, Japan
Apweiler, Rolf	European Bioinformatics Institute, United Kingdom
Armstrong, Neal	University of Arizona
Arnold, Frances	California Institute of Technology
Atkins, Peter	University of Oxford, United Kingdom
Attfield, Paul	University of Edinburgh, United Kingdom
Baba, Yoshinobu	Nagoya University, Japan
Backvall, Jan-E.	Stockholm University, Sweden
Baer, Eric	Case Western Reserve University
Balzani, Vincenzo	University of Bologna, Italy
Barbara, Paul	University of Texas
Barrett, David	University of Nottingham, United Kingdom
Bartlett, Rodney J.	University of Florida
Barton, Jacqueline K.	California Institute of Technology
Bell, Alexis	University of California, Berkeley
Bergman, Robert	University of California, Berkeley
Bernasek, Steven L.	Princeton University
Bernath, Peter	University of Waterloo, Canada
Berry, R. Stephen	University of Chicago
Bertozzi, Carolyn	University of California, Berkeley
Binder, Kurt	Johannes Gutenberg University, German
Birk, James	Arizona State University
Bochmann, Manfred	University of East Anglia, United Kingdom
Bodner, George	Purdue University
Boxer, Steven G.	Stanford University
Braga, Dario	University of Bologna, Italy
Breslow, Ronald	Columbia University
Brinker, Jeffrey	Sandia National Laboratory
Brunelle, Daniel J.	GE Global Research
Campbell, Charles	University of Washington
Campbell, Simon	Pfizer (retired)
Cantor, Charles	Boston University
Car, Roberto	Princeton University
Carpenter, Barry	Cornell University
Caruso, Frank	University of Melbourne, Australia
Casavecchia, Piero	University of Perugia, Italy
Cava, Robert	Princeton University
Cech, Thomas	University of Colorado, Boulder

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TABLE D-2 Continued

Name	Affiliation
Chandler , David	Sandia National Laboratory
Chang, Bor-Chen	National Central University, Taiwan
Cheng, Stephen Z.	University of Akron
Chiang, Shirley	University of California, Davis
Chorkendorff, Ib	Danish National Research Foundation, Denmark
Christe, Karl	University of Southern California
Clardy, Jon	Harvard University
Clark, David	Los Alamos National Laboratory
Clary, David	University of Oxford, United Kingdom
Coates, Geoffrey	Cornell University
Colby, Ralph	Pennsylvania State University
Continetti, Bob	University of California, San Diego
Cooks, Graham	Purdue University
Cordell, Geoffrey	University of Illinois, Chicago
Corn, Robert	University of California, Irvine
Cossy, Janine	École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, France
Crim, F. Fleming	University of Wisconsin, Madison
Crowley, John	Max Planck Institute for Chemistry, Germany
Dai, Hai-Lung	University of Pennsylvania
Danishefsky, Samuel	Columbia University
Dantus, Marcos	Michigan State University
Davis, Benjamin	University of Oxford, United Kingdom
Davis, Mark	California Institute of Technology
de Jong, Onno	Utrecht University, Netherlands
de Meijere, Armin	University of Goettingen, Germany
Decher, Gero	Université Louis Pasteur, France
Decicco, Carl	Bristol-Myers Squibb
DeSimone, Joseph M.	University of North Carolina, Chapel Hill
Dickson, Robert	Georgia Institute of Technology
Diederich, Francois	ETH Zurich, Switzerland
Dill, Kenneth	University of California, San Francisco
Ding, Yu-Shin	Yale University
DiSalvo, Frank	Cornell University
Dixneuf, Pierre	University of Rennes, France
Dougherty, Dennis	California Institute of Technology
Dovichi, Norm	University of Washington
Driess, Matthias	Technical University of Berlin, Germany
Duncan, Michael	University of Georgia
Ebata, Takayuki	Hiroshima University, Japan
El-Sayed, Mostafa	Georgia Institute of Technology
Enders, Dieter	Aachen University, Germany
Erker, Gerhard	University of Muenster, Germany
Evans, David A.	Harvard University
Ewing, Andrew	Pennsylvania State University
Faber, Kurt	University of Graz, Austria
Fahmy, A.F.M	Ain Shams University, Egypt

continued

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TABLE D-2 Continued

Name	Affiliation
Fayer, Michael	Stanford University
Field, Robert	Massachusetts Institute of Technology
Fischer, Edmond	University of Washington
Flaud, Jean-Marie	Centre National de la Recherche Scientifique, France
Fleming, Graham	University of California, Berkeley
Flitsch, Sabine	University of Manchester, United Kingdom
Francis , A.J.	Brookhaven National Laboratory
Frenkel, Daan	University of Amsterdam, Netherlands
Freund, Hans-Joachim	Fritz Haber Institute, Germany
Galli, Giulia	Lawrence Livermore National Laboratory
Gates, Bruce	University of California, Davis
Gerber, Gustav	University of Wurzburg, Germany
Gibson, Harry	Virginia Polytechnic Institute and State University
Gorte, Ray	University of Pennsylvania
Gray, Harry B.	California Institute of Technology
Griesinger, Christian	Max Planck Institute for Biophysical Chemistry, Germany
Griffin, Robert G.	Massachusetts Institute of Technology
Grunze, Michael	University of Heidelberg, Germany
Hacksell, Uli	ACADIA Pharmaceuticals
Hahn, Richard	Brookhaven National Laboratory
Halberstadt, Nadine	Universite Paul Sabatier Toulouse III, France
Hamers, Bob	University of Wisconsin, Madison
Harada, Akira	Osaka University, Japan
Harrison, Jed	University of Alberta, Canada
Hartwig, John	University of Illinois, Urbana-Champaign
Hauer, Bernard	BASF, Germany
Haueter, Max	ETH Institute of Molecular Systems Biology, Switzerland
Hawker, Craig	University of California, Santa Barbara
Hayashi, Tamio	University of Kyoto, Japan
Healy, Kevin	University of California, Berkeley
Heard, Dwayne	University of Leeds, United Kingdom
Hemminger, John	University of California, Irvine
Heeren, Ronald	Institute for Atomic and Molecular Physics, Netherlands
Herrmann, Hartmut	Leibniz Institute for Tropospheric Research, Germany
Hines, Melissa	Cornell University
Hochstrasser, Robin	University of Pennsylvania
Hoffmann, Peter	University of Heidelberg, Germany
Horwich, Arthur	Yale University
Houk, Kendall N.	University of California, Los Angeles
Houston, Paul	Cornell University
Hovis, Jennifer	Purdue University
Hsieh, Linda	California Institute of Technology
Hubbell, Jeffrey	ETH, Zurich, Switzerland
Hutchings, Graham	Cardiff University, United Kingdom
Hutchinson, Richard	Kosan Biosciences
Iglesia, Enrique	University of California, Berkeley
Ireland, Chris	University of Utah

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TABLE D-2 Continued

Name	Affiliation
Ismasgilov, Rustem	University of Chicago
Iwasawa, Yasuhiro	University of Tokyo, Japan
Jaeger, Wolfgang	University of Alberta, Canada
Janda, Kenneth C.	University of California, Irvine
Jonas, David	University of Colorado, Boulder
Jorgensen, Karl A.	University of Aarhus, Denmark
Jorgensen, William L.	Yale University
Jortner, Joshua	Tel Aviv University, Egypt
Joyce, Gerald	Scripps Research Institute
Jurisson, Silvia	University of Missouri, Columbia
Kanatzidis, Mercouri	Michigan State University
Karlin, Kenneth D.	Johns Hopkins University
Kay, Bruce	Pacific Northwest National Laboratory
Kennedy, Robert T.	University of Michigan
Kiessling, Laura	University of Wisconsin, Madison
Kiick, Kristi	University of Delaware
Kilbourn, M.	University of Michigan
Kira, Mitsuo	Tohoku University, Japan
Klein, Michael L.	University of Pennsylvania
Klibanov, Alexander	Massachusetts Institute of Technology
Knowles, Jeremy	Harvard University
Kolb, Dieter	University of Ulm, Germany
Korgel, Brian	University of Texas
Krauss, Todd D.	University of Rochester
Krausz, Ferenc	Max Planck Institute for Quantum Optics
Kremer, Kurt	Max Planck Institute for Chemistry
Krogsgaard-Larsen, Povl	Carlsberg Foundation, Denmark
Kung, Hank	University of Pennsylvania
Kung, Harold	Northwestern University
Lagowski, Joseph J.	University of Texas
Langer, Robert	Massachusetts Institute of Technology
Langstrom, Bengt	Uppsala University, Sweden
Larson, Ron	University of Michigan
Lee, Ka Yee	University of Chicago
Lehmann, Kevin	University of Virginia
Leigh, David	University of Edinburgh, United Kingdom
Lester, William	University of California, Berkeley
Levy, Donald H.	University of Chicago
Ley, Steven	University of Cambridge, United Kingdom
Li, Can	Chinese Academy of Sciences, China
Lippard, Steven	Massachusetts Institute of Technology
List, Benjamin	Max Planck Institute for Bioinorganic Chemistry
Liu, Kopin	Academia Sinica, China
Lunsford, Jack	Texas A&M University
Lyon, L. Andrew	Georgia Institute of Technology
MacMillan, David	California Institute of Technology
MacPherson, Julie V.	University of Warwick, United Kingdom

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Name	Affiliation
Maier, John Paul	University of Basel, Switzerland
Mallouk, Thomas E.	Pennsylvania State University
Mann, Matthias	Max Planck Institute of Biochemistry, Germany
Mann, Stephen	University of Bristol, United Kingdom
Manthe, Uwe	University of Bielefeld, Germany
Manz, Andreas	Institute for Analytical Sciences, Germany
Martel, Richard	University of Montreal, Canada
Martin, Jean-Louis	Centre National de la Recherche Scientifique, France
Martinez, Jean	University of Montpellier, France
Maruoka, Keiji	University of Kyoto, Japan
Mathey, Francois	University of California, Riverside
Matsui, Hiroshi	City University of New York
Matsushima, Tatsuo	Hokkaido University, Japan
Mavrikakis, Manos	University of Wisconsin, Madison
Mays, Jimmy W.	University of Tennessee
McLeish, Tom	University of Leeds, United Kingdom
Meares, Claude	University of California, Davis
Meijer, E. W. (Bert)	Eindhoven University of Technology, Netherlands
Merer, Anthony	University of British Columbia, Canada
Merkt, Frederic	ETH Zürich, Switzerland
Meyerhoff, Mark	University of Michigan
Michl, Josef	University of Colorado, Boulder
Miller, Terry	Ohio State University
Mirkin, Chad	Northwestern University
Mitscher, Lester	University of Kansas
Moody , Kenneth	Lawrence Livermore National Laboratory
Mooney, David	Harvard University
Moore, Peter	Yale University
Moore, Robert	University of Southern Mississippi
Morokuma, Keiji	Emory University
Morse, Daniel	University of California, Santa Barbara
Muller-Dethlefs, Klaus	University of Manchester, United Kingdom
Mulvaney, Paul	University of Melbourne, Australia
Murray, Royce	University of North Carolina, Chapel Hill
Nakanishi, Koji	Columbia University
Nathanson, Gilbert M.	University of Wisconsin, Madison
Nelson, Keith	Massachusetts Institute of Technology
Nicolaou, K.C.	Scripps Research Institute
Niessner, Reinhard	Technical University of Munich, Germany
Norris, David	University of Minnesota, Twin Cities
Norskov, Jens K.	Technical University of Denmark
Novotny, Lukas	University of Rochester
Nozik, Arthur	National Renewable Energy Laboratory
Nuzzo, Ralph	University of Illinois, Urbana-Champaign
Nyman, Gunnar	Goteborg University, Sweden
Ober, Christopher K.	Cornell University
Oka, Takeshi	University of Chicago
Okumura, Mitchio	California Institute of Technology

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Name	Affiliation
Orr-Ewing, Andrew	Bristol University, United Kingdom
Ozin, Geoffrey	University of Toronto, Canada
Pak, Young-Ki	Yonsei University, Korea
Panagiotopoulos, Athanassios Z.	Princeton University
Parker, David H.	Radboud University Nijmegen, Netherlands
Pecec, Virgil	University of Pennsylvania
Petek, Hrvoje	University of Pittsburgh
Petsko, Gregory	Brandeis University
Piers, Warren	University of Calgary, Canada
Pileni, Marie-Paule	University of Pierre and Marie Curie, France
Pochan, Darrin	University of Delaware
Poulter, Dale	University of Utah
Prins, Roel	ETH Zürich, Switzerland
Prisner, Thomas	University of Frankfurt, Germany
Pyykko, Pekka	University of Helsinki, Finland
Rabani, Eran	Tel Aviv University, Egypt
Radom, Leo	University of Sydney, Australia
Ramsey, Michael	University of North Carolina, Chapel Hill
Ratnasamy, Paul	National Chemical Laboratory, India
Ratner, Buddy D.	University of Washington
Ravishankara, A.R.	National Oceanic and Atmospheric Administration, Aeronomy Laboratory
Raymond, Kenneth N.	University of California, Berkeley
Reedijk, Jan	Leiden University, Netherlands
Rees, Douglas C.	California Institute of Technology
Reetz, Manfred	Max Planck Institute for Bioinorganic Chemistry, Germany
Reineke, Theresa	University of Cincinnati
Rich, Daniel H.	University of Wisconsin, Madison
Richards, Graham	University of Oxford, United Kingdom
Robb, Michael	Imperial College London, United Kingdom
Robinson, William	Purdue University
Roethlisberger, Ursula	Swiss Federal Institute of Technology, Lausanne
Roncero, Octavio	CSIC, Spain
Roos, Bjorn	Lund University, Sweden
Rowan, Stuart J.	Case Western Reserve University
Runde , Wolfgang	Los Alamos National Laboratory
Ruth, Thomas J.	University of British Columbia, Canada
Sander, Wolfram	Ruhr University Bochum, Germany
Saykally, Richard	University of California, Berkeley
Scheffler, Matthias	Fritz Haber Institute, Germany
Schimmel, Paul	Scripps Research Institute
Schriner, Peter	Justus Liebig-Universität Gießen, Germany
Schulten, Klaus	University of Illinois, Urbana-Champaign
Schultz, Peter	Scripps Research Institute
Scoles, Giacinto	Princeton University
Seeman, Nadrian C.	New York University

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Name	Affiliation
Sekiguchi, Akira	University of Tsukuba, Japan
Shore, Sheldon	Ohio State University
Sibener, Steven J.	University of Chicago
Simpson, Richard	Australia
Singleton, Daniel	Texas A&M University
Sneddon, Larry G.	University of Pennsylvania
Snieckus, Victor	Queens University, Canada
Soep, Benoit	CEA, Saclay, France
Solomon, Edward	Stanford University
Sprik, Michiel	University of Cambridge, United Kingdom
Springer, Charles	Oregon Health and Science University
Stair, Peter	Northwestern University
Stang, Peter	University of Utah
Stolto, Steve	Vrije University, Netherlands
Stone, Morley	Defense Advanced Research Projects Agency
Stroscio, Joseph	National Institute of Standards and Technology
Stucky, Galen	University of California, Santa Barbara
Stupp, Samuel I.	Northwestern University
Suzuki, Toshinori	RIKEN, Japan
Sweedler, Jonathan	University of Illinois, Urbana-Champaign
Takada, Shoji	Kobe University, Japan
Taylor, Susan	University of California, San Diego
Thiel, Patricia A.	Iowa State University
Tijan, Robert	University of California, Berkeley
Tilley, T. Don	University of California, Berkeley
Tirrell, David	California Institute of Technology
Tokmakoff, Andrei	Massachusetts Institute of Technology
Tolman, William	University of Minnesota, Twin Cities
Topsoe, Henrik	Haldor Topsoe, Denmark
Trost, Barry M.	Stanford University
Tuross, Noreen	Harvard University
Utz, Arthur L.	Tufts University
Vaccaro, Patrick H.	Yale University
van Leeuwen, Piet	University of Amsterdam, Netherlands
van Santen, Rutger	Eindhoven University of Technology, Netherlands
Vogel, Viola	ETH, Zürich, Switzerland
Voit, Brigitte	Institute for Polymer Research, Dresden, Germany
Vorhees, Kent	Colorado School of Mines
Wagener, Ken	University of Florida
Waldmann, Herbert	Max Planck Institute of Molecular Physiology, Germany
Walt, David	Tufts University
Wang, Hongfei	Chinese Academy of Sciences, China
Wang, James	Pennsylvania State University
Ward, Michael	New York University
Weber, Peter	Brown University
Weckhuysen, Bert	Utrecht University, Netherlands
Weighardt, Karl	Max Planck Institute for Bioinorganic Chemistry, Germany

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Name	Affiliation
Weiner, Steve	Weizmann Institute of Science, Israel
Weiss, Shimon	University of California, Los Angeles
Welch, Michael	University of Washington
Weller, Horst	University of Hamburg, Germany
Wells, James	University of California, San Francisco
Whitesides, George M.	Harvard University
Williams, R.J.P.	Northwestern University
Williams, Stan	Hewlett Packard Laboratories
Wodtke, Alec	University of California, Santa Barbara
Wolynes, Peter	University of California, San Diego
Wooley, Karen	University of Washington
Wudl, Fred	University of California, Los Angeles
Yamato, Masayuki	Tokyo Women's Medical University, Japan
Yamamoto, Hisashi	University of Chicago
Yang, Dan	University of Hong Kong
Yang, Peidong	University of California, Berkeley
Yang, Xueming	Dalian University of Technology, China
Yates, John	Scripps Research Institute
Yates, Steven W.	University of Kentucky
Yurke, Bernard	Bell Labs, Lucent Technologies
Zaera, Francisco	University of California, Riverside
Zare, Richard	Stanford University
Zasadzinski, Joseph	University of California, Santa Barbara

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