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Product Specifications Page 14 Share Cite Suggested Citation:"2 Key Characteristics of U.S. Chemistry Research." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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.) 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- Page 2 Page 20 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 Page 21 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 22 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 23 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 24 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 25 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × FIGURE 3-2 Comparison of select country and regional production of chemistry papers, 1996 to June 2006. SOURCE: Thomson ISI Essential Science Indicators. Central/S 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. Page 26 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 27 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 28 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 29 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × FIGURE 3-8 Research portfolio of China, 1996 and 2003. 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. 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 Page 30 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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- Page 31 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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). Page 32 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 33 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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.) Page 34 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. 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 U.S. %, Most Highly Cited by Area 1990-1994 1995-1999 2000-2006 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 Page 35 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 36 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 37 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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). Page 38 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. 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 Page 39 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 40 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. This section looks more closely at the different areas and subareas in which chemists classify their research. These areas were chosen by the panel Page 41 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 42 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 (. 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 (. 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 (or , 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 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 Page 43 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 44 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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- Page 45 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 Page 46 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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

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 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 Page 56 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 57 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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- Page 58 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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. Page 59 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 Page 60 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 Page 61 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 62 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 63 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 C60, 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. Page 64 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 65 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Ultrafast spectroscopy primarily employs optical techniques to study molecular motion in the femtosecond to attosecond range. 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- Page 66 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 Page 67 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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 Page 68 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × structure simulation and computer-aided chemical discovery. No papers from basic theory development were among the 100 hot articles. 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. The United States is the leader in analytical chemistry, biological chemistry, chemistry education, inorganic chemistry, and in materials chemistry and nanoscience. Page 69 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 20 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 21 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 22 Share Cite Suggested Citation:"3 Current Research Leadership Position." 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National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 47 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 48 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 49 Share Cite Suggested Citation:"3 Current Research Leadership Position." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 50 Share Cite Suggested Citation

magnetic resonance Mass spectrometry Cyber-enabled chemistry Chemical biology Reactors and accelerators 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- Page 80 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Appleton Laboratories in the United Kingdom; and the Hi-Flux Advanced Neutron Application Reactor in Korea.7 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 (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 (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 ( ) 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 (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- Page 81 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × versity Nanofabrication Facility,8 which are available to external users and are part of a larger National Nanotechnology Infrastructure Network. 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. 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. NSF defines cyber-infrastructure as the distributed computer, information, and communication technologies combined with the personnel and Page 82 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 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, (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 Page 83 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 (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. 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 Page 84 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 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. 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. Page 85 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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, 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 Page 86 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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- Page 87 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 88 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 89 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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), (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- Page 90 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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). Page 91 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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), (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. Employment of chemistry degree holders has steadily increased over the years (see Figure 4-13). The percent change from 1999 to 2003 was Page 92 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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), (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 Page 93 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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), (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: Page 94 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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), (accessed September 25, 2006). Data from the American Chemical Society15 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 Page 95 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 96 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × FIGURE 4-14 Comparison of employed chemistry degree holders across different sectors, 1999 and 2003. SOURCE: Science and Engineering 2004, 2006. 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. 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 Page 97 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 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 Page 98 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 different federal agency contributions to the total funding for both nonacademic and academic chemistry research are shown in Figure 4-24. Page 99 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Median annual salaries of U.S. che 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. Page 100 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 101 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 102 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 103 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 104 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 105 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 106 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 107 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 (accessed October 5, 2006). Page 108 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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.) 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 (assessed October 6, 2006). Page 109 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. Page 110 Share Cite Suggested Citation:"4 Key Factors Influencing Leadership." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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

10.17226/11866. × Page 135 Share Cite Suggested Citation:"C Journal Analysis." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 136 Share Cite Suggested Citation:"C Journal Analysis." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Page 8 Page 137 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × Appendix D Virtual World Congress FIGURE D-1 Virtual world congress organizers by area of chemistry and U.S. residency. Page 138 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × TABLE D-1 Detailed Results for Chemistry Virtual Congress Area Subarea Organizers No. of Organizers U.S. Non-U.S. % 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 Page 139 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 140 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 141 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 142 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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 Page 143 Share Cite Suggested Citation:"D Virtual World Congress." National Research Council. 2007. The Future of U.S. Chemistry Research: Benchmarks and Challenges. Washington, DC: The National Academies Press. doi: 10.17226/11866. × 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. 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