CAN THE U.S. COMPETE *in Basic Energy Sciences?*

CRITICAL RESEARCH FRONTIERS AND STRATEGIES

A report by the BESAC Subcommittee on International Benchmarking

Front and back covers depict the most accurate flat map of Earth yet (by J. Richard Gott, David Goldberg, and Robert Vanderbei). It's a revolutionary two-sided map like a vinyl phonograph record: northern hemisphere on one side, southern hemisphere on the other, with the equator running around the edge. It minimizes distortions, distance errors, and discontinuities.

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Critical Research Frontiers and Strategies

A report by the BESAC Subcommittee on International Benchmarking

2021

Department of Energy
Office of Science
Washington, DC 20585

February 5, 2019

Dr. Marc Kastner
Science Philanthropy Alliance
480 S. California Avenue #304
Palo Alto, California 94306

Dear Dr. Kastner:

I very much appreciate your assuming the position of Chair of the Basic Energy Sciences Advisory Committee (BESAC). I also want to express my sincere appreciation for your past contributions to BESAC, especially for your leadership on the BESAC "BES40" Subcommittee culminating in the completion of the excellent BESAC report *A Remarkable Return on Investment in Fundamental Research*, commemorating the 40th anniversary of the Basic Energy Sciences (BES) program.

As illustrated in the BES40 report, sustained federal support through BES has shaped the field of research, opened new lines of scientific inquiry, and led to inventions of new technologies and industries that transformed our society. The successes captured in the report reflect the vibrant national Science & Technology innovation environment, which has been the model emulated throughout the rest of the world in the past half century.

Specifically, the BES40 report affirmed the distinctive community-driven strategic planning process that has been used to identify and implement the most compelling and impactful early-stage basic research opportunities for the nation. It further highlighted the BES-created large scale scientific user facilities at the frontiers of physics, chemistry, materials science, and biology. The single Recommendation from the BES40 report asked BES to be bold in choosing new research and facilities to support and experimenting with new funding mechanisms where appropriate.

This recommendation is especially timely in view of intensifying globalization in research talent and resources. In pursuing additional research, facility, and funding mechanisms to support, I am writing to ask BESAC to provide input on possible implementation strategies, especially in the context of keeping pace with international competition.

I ask BESAC to consider the following questions in formulating the study plan:

- Within the BES-supported topical research areas and facility capabilities, in which areas and capabilities is U.S. leadership most threatened, presently or in the foreseeable future? Consider their critical mission relevance, recent history, the status quo, observable trends, and evidence-based projections.

- To preserve and foster U.S. leadership with resource constraints, what are the key efficiencies and balances that should be sought? Should the existing trade-offs in BES be modified in some of these critical areas? Can resources be leveraged in new ways, through collaborations within and beyond the BES research and facility communities?

- For someone deciding whether to pursue a scientific career, or a mature scientist considering whether to stay in the U.S., how can BES programs and facilities be structured and managed to create incentives that will attract and retain talented people? What are the key attractions and deterrents of a career in BES-supported science areas? How can the mix of research funding modalities be designed to enhance the attractions and minimize the deterrents?

I would appreciate receiving a written report by July 31, 2020.

Sincerely,

J. Stephen Binkley
Deputy Director for Science Programs
Office of Science

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EXECUTIVE SUMMARY

Scientific discovery is a cornerstone of American prosperity. It is nearly impossible to imagine any aspect of our work and our lives that has not been touched, shaped, and enhanced by science and technology. For more than 75 years, our national investment in American science and scientists has yielded incalculable dividends for our country. In particular, basic scientific research, which is driven by the desire to understand fundamental principles, often leads to unexpected discoveries. These in turn provide the basis for innovation and technical developments: indeed, many of today's most important technologies originated in U.S. basic research from decades past.[1] Without continued investment in basic science today, future discoveries and technological innovation will languish.

That is a real concern, because there is ample evidence in this and other reports that the United States is falling behind other countries in such investments.[2] For example, China is on pace to surpass the United States in spending on research and development, putting America in second place for the first time in a century. Other nations are also building next-generation research tools and providing substantial, long-term support for programs large and small. Indeed in 2020, as measured by investment in scientific research and development as a fraction of GDP, the U.S. ranked only 10th in the world.[2] Equally important is the ability to compete for scientific talent. In decades past U.S. research experience was considered essential for any ambitious young scientist and drew thousands of highly talented individuals, many of whom ultimately chose to stay and pursue their careers as Americans. Now, however, the diminished U.S. capability to attract and retain international talent is reflected in the falling numbers of foreign students, postdocs, and early career scientists who choose to study and work in U.S. universities and laboratories.[2]

While the increased investment in basic science worldwide will have a positive impact on humankind overall, it is clear that the U.S. scientific enterprise has reached an historic crossroad. With investments in scientific infrastructure and education increasing around the world, the era of unquestioned American scientific dominance is drawing to a close. Our challenge now is to focus on those critical areas in which we can and must achieve U.S. leadership, including building a robust, diverse scientific workforce, in order to drive durable economic growth and to address the grand challenges in energy, environment, and national security that will shape our nation for decades to come.

In light of these concerns, the Basic Energy Sciences Advisory Committee (BESAC) has been charged by the Office of Science of the U.S. Department of Energy (DOE) to identify critical research areas in basic energy sciences; to examine U.S. competitiveness in these areas, in major research facilities and tools, and in funding mechanisms; and to suggest strategies that could enhance the U.S. position in comparison to its global competitors.

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1. "A Remarkable Return on Investment in Fundamental Research. 40 Years of Basic Energy Sciences at the Department of Energy" (U.S. Department of Energy, Office of Science, 2018), www.science.osti.gov/-/media/bes/pdf/BESat40/BES_at_40.pdf

2. *The Perils of Complacency, America at a Tipping Point in Science and Engineering* (American Academy of Arts and Sciences, 2020), www.amacad.org/publication/perils-of-complacency

Critical Areas for Basic Energy Research

This report focuses on five forward-looking critical areas in which other nations are investing heavily and are constructing and upgrading facilities to achieve technical quality similar to that of the United States but with greater experimental capacity. These are not the only areas of importance, but they illustrate the challenges across many sectors of basic energy research. For each selected area and selected sub-fields, this report provides both a detailed description and quantitative evidence of the competitive landscape, as well as relevant examples of recent or on-going research that illustrates their social, economic, or strategic importance. These selected critical areas, in brief, comprise:

1. ***Quantum Information Science***, which includes quantum algorithms, quantum computing, quantum communications, and related areas.
2. ***Science for Energy Applications***, which includes energy storage, membranes, and sustainable fuels.
3. ***Matter for Energy and Information***, which includes quantum materials, nanoscience and neuromorphic computing.
4. ***Industrially-relevant Science for Sustainability***, which includes carbon capture, chemical upcycling of plastics, transformative manufacturing, and other areas.
5. ***Advanced Research Facilities***, a cross-cutting area that includes synchrotron and free-electron X-ray sources, reactor and spallation neutron sources, electron microscopy facilities, nano-scale research centers, and high-performance computing. These facilities have played a critical role in the advance of both basic and applied science through their ability to analyze the structure and properties of materials. So important are such research tools that there is world-wide competition for access to the latest, most powerful facilities. As this report documents, here too the U.S. is in many aspects falling behind.

For each of these critical areas of research, this report finds compelling evidence that China's progress is surging and that Europe leads in quantum information sciences, while U.S. research output is flattening or falling behind.

Strategies for Success

Improving U.S. competitiveness in basic energy sciences seems imperative. To do so, this report recommends consideration of four broad strategies:

- Increase investment in basic energy sciences research, including the development of research programs and advanced research facilities and instrumentation at both universities and national labs.
- Boost support for early-career and mid-career scientists to levels comparable to leading programs elsewhere, so as to better attract and retain talent.
- Enhance opportunities for staff scientists at advanced research facilities, to provide more scope for their own scientific careers and retain their talent, and to unleash their creativity for instrumentation development and other facility improvements.
- Better integrate energy sciences research across the full spectrum—from basic to applied to industrial research.

KEY FINDINGS AND RECOMMENDATIONS

The overall trend in all research areas identified in this report as critical to the Department of Energy's Office of Basic Energy Sciences mission is a downward trend in the U.S. competitive advantage starting about 2010 and continuing to the present. An important driver of this trend is the significantly increased investment in basic research in Asia and Europe. While the U.S. leadership position in the specific critical research areas investigated in this report varies in detail, the trend is clear—increased investment by other countries is having a major impact. China's investment has been particularly strong in the past decade. At the same time, U.S. funding for research has been relatively flat, resulting in a loss of leadership in many of these fields. The consequences of these changes on our society will become evident with time since basic research is the "seed corn" of new technologies.

An important component of scientific leadership is the availability of world-class research facilities both at universities and at national labs. The advanced research facilities in the U.S. funded by DOE's Office of Basic Energy Sciences are world leading, if no longer unique, largely because of long-range strategic planning, ongoing stewardship, and investment. There are many examples of highly impactful work performed at such large-scale facilities, including multiple Nobel Prizes, as described later in this report. At the same time, continuous long-term planning and financing is required to remain at the top, creating a need for the future. While facilities in the U.S. set the pace technically, demand for access to them far exceeds their current capacity; access to comparable facilities is more extensive in other countries, especially in Europe. Additionally, supporting resources such as the number of staff scientists available to assist both university and industrial users of these complex facilities are more extensive outside the U.S.

Development of mid- and small-scale instrumentation by individual or small groups of scientists is another cornerstone of fundamental energy science. Design and building of new instruments to address specific fundamental science questions in individual laboratories has historically led to both scientific breakthroughs and ultimately new tools used for applications that benefit society. There are many historical examples, such as development of magnetic resonance imaging that grew out of fundamental research in physics and nuclear magnetic resonance to become a key medical technology; it is now also used in many industrial applications. But support for development of new instrumentation is increasingly difficult to obtain in the U.S.

The increasing importance of computation and data analysis in fundamental and applied sciences leads to another concern about U.S. leadership. New hardware and software—computer codes and algorithms including artificial intelligence and machine learning—are critical to advancing both science and technology. The U.S. is not in a leading position overall in these areas, creating a concern for future national security and leadership in science and engineering.

The U.S. is also losing ground in the competition for global talent. Attracting global talent has historically been important to leadership in fundamental science worldwide. Furthermore, the U.S. was long considered a destination for international scientists seeking a successful career. The investment in science in other countries, including resources available for research as well as freedom to travel and exchange ideas, have changed the landscape so that the U.S. is no longer automatically the preferred destination for career development.

The translation of fundamental research to technological applications is a long-term process that could usefully be accelerated to address many pressing problems facing society. As the pandemic has made clear and looming climate challenges suggest, we often need more rapid solutions—years or months, instead of decades. To that end there is a need to facilitate overlapping or simultaneous stimulation of basic research, use-inspired research, applied research and industrial research that would invigorate innovation and shorten the time from fundamental discovery to application and implementation.

Overall, the key findings of this report are that investment in basic energy sciences research and instrumentation, long-term strategic planning, talent development and retention, and better integration across the spectrum of fundamental to applied research are critical components of U.S. competitiveness now and in the future.

Recommendations

There are clearly many areas of concern to potentially be addressed in the future if the U.S. is to maintain a leadership role in critical areas of science. A balance of investments will be required to optimize the impact of scientific work in areas of research essential to the Department of Energy mission. Based on the findings in this report, we offer several recommendations that have the potential for significant societal impact in the future.

- Stronger investments in advanced research infrastructure, including laboratory-based and large-scale instrumentation, would bolster U.S. competitiveness.
- Striking a balance between the need to develop world-leading facilities and the need for access to and technical support of existing facilities would increase research impact and help retain talented scientists.
- Mechanisms for significant financial support of scientific investigators at all career stages would create a more sustainable career path that builds on current investments in the development of the scientific workforce—enhancing U.S. competitiveness for talent.
- Additional investment in computational and data analysis methods and computer hardware and architecture has major potential in basic research and future applications.
- Enhanced international cooperation in selected areas has the potential to enhance U.S. competitiveness.
- Facilitation of interaction across the continuum of basic research, use-inspired research, applied research and industrial research could accelerate translation of fundamental research to impactful technologies that benefit society.

INTRODUCTION

In preparing this report, the subcommittee identified five broad areas of critical scientific research. These choices are not a comprehensive list, but are rather exemplary of the competitiveness challenges facing many of the activities that fall within the purview of the DOE Office of Basic Energy Sciences. The subcommittee then pursued several sources of data—including citations in the scientific literature and invited presentations at major scientific conferences—that would allow it to provide evidence-based conclusions about U.S. competitiveness in these areas. The report includes examples of the relevant data, and more complete detail in the Appendix. The subcommittee also consulted many leading scientists as a basis for identifying issues related to U.S. competitiveness—including funding mechanisms, the global competition for scientific talent, and capacity limits on access to major research facilities—and potential remedies for these issues.

In addition, the subcommittee sought out specific examples of research in the critical areas identified that could illustrate both the social and economic benefits of such research, and also some of the constraints and challenges facing U.S. science and scientists. The report includes non-technical descriptions of these examples, many of which put a human face on the science.

The picture that emerges from these investigations is complex but unambiguous: U.S. scientific leadership—both in the critical areas identified and more broadly—is now strongly challenged, and the ability to compete internationally is at risk.

In many respects, the Nation is now at a generational inflection point that mirrors the situation that faced Vannevar Bush, the director of U.S. Office of Scientific Research and Development, in 1945. At that time, America was just beginning to recover from the dual cataclysms of the Great Depression and World War II. Yet when he published *Science: The Endless Frontier*, his blueprint for organizing government support of scientific research, Bush did not flinch from calling for massive new science investments. Today, it is clear that Bush's ambitious vision yielded extraordinary scientific results and unprecedented economic expansion for the United States. That vision has informed the important and successful work of the U.S. Department of Energy's Office of Basic Energy Sciences over the past decades, and it continues to inspire as we confront the challenges of our own time.

With this report, the Committee hopes to stimulate a new and potentially transformational national conversation. The Office of Basic Energy Sciences is in a strong position to make thoughtful, targeted decisions about where the United States should collaborate and where we should compete in this new, global marketplace of scientific exploration and discovery. By focusing our sights, forging productive new collaborations, and making strategic investments, we can restore and preserve U.S. scientific leadership in the critical areas described here while strengthening our research infrastructure and training a large, more diverse generation of scientists—thus paving the way to a prosperous, secure American future.

To fulfill this promise will require substantial, expanded investments, as well as innovative policies and programs. This Committee is keenly aware that we make these recommendations and call for these actions in a time of constrained federal resources. We understand that a seemingly endless array of worthy and conflicting priorities must be balanced by the Nation's leaders. We also understand the need to leverage resources in new ways and to seek efficiencies in facilities and operations. But we cannot allow these realities to limit our imaginations nor to mute our advocacy. The DOE Office of Basic Energy Sciences is a pillar of the U.S. research infrastructure with a duty to pursue its mission—including funding basic energy science and the advanced research facilities such research requires—with zeal and determination.

Yet fulfilling the responsibility of the scientific enterprise to the nation will require more than development and publication of a thoughtful, well-articulated list of goals, priorities, and recommendations. The Office of Basic Energy Sciences also has the opportunity to expand on its bold vision of scientific leadership. When this tragic pandemic comes to a close, we face an unprecedented and unexpected opportunity to recapture the public imagination. A year ago, it would have been unimaginable that millions of Americans would be sharing scientific studies on Facebook and delving into the nuances of gold-standard research design and sample size. The incredibly swift development of novel and effective coronavirus vaccines, based on a completely new methodology developed through basic research, has forcefully demonstrated the power of science to save lives and change history. This achievement has opened a brief window of public attention, creating an opportunity to expand awareness of how basic science provides the foundation of future innovation and applications that will have a positive impact on our society.

1. CRITICAL SCIENTIFIC AREAS FOR LEADERSHIP IN BASIC ENERGY SCIENCES

Overview

While the U.S. has long been the leader in areas of research critical to basic energy sciences, other nations are rapidly catching up and overtaking the U.S. The emergence of Asian and European leadership in specific subfields corresponds to a period of rapid growth in research investment by China and to a lesser extent in Europe, along with a flattening of U.S. investment in science and technology.

Methodology

Five broad areas were identified as critical fundamental scientific topics for leadership in basic energy sciences. These areas were identified through an analysis of publicly available BESAC reports and DOE Office of Basic Energy Sciences Basic Research Needs (BRN) reports from 2010 onward (see Appendix). The BRN reports are strategically aligned with basic energy science priorities. The five critical scientific areas identified from the committee review are summarized in Table 1. The Committee recognizes that these five topics will likely evolve and that new topics will arise with future discoveries and innovations. Tools and advanced research facilities are of particular importance to the BES mission and have a crosscutting impact in all science areas. In alignment with the committee charge, only basic scientific research prioritized by the Office of Basic Energy Sciences was considered for this report; however, it is likely that the broad trends will apply to other fields of interest in energy science. All areas identified have potentially significant impacts on U.S. innovation and technology development in the future.

TABLE 1. Five Areas Identified as Critical to the BES Mission with Selected Subareas

	AREAS	SUB-AREAS
1	**Quantum Information Science**	Quantum computation, quantum communication, quantum simulation, quantum sensing
2	**Science for Energy Applications**	Membranes, interfaces, energy storage, sustainable fuels
3	**Matter for Energy and Information**	Quantum materials, mesoscience, nanoscience, neuromorphic computing
4	**Industrially-Relevant Science for Sustainability**	Chemical upcycling of polymers, electrocatalysis, carbon capture, transformative manufacturing
5	**Advanced Research Facilities**	Neutron sources, synchrotron and free electron laser X-ray sources, electron microscopy

The committee consulted BESAC BRN report leads on the status of the respective fields. Using this input and expertise within the sub-committee (see Appendix for more details), a few sub-topics were selected for an in-depth analysis: i) quantum algorithms, quantum computation; ii) membranes, interfaces, sustainable fuels; iii) quantum materials, meso-science, nanoscience, neuromorphic computing; iv) chemical upcycling of polymers, electrocatalysis, carbon capture, transformative manufacturing; v) Synchrotron and free electron laser X-ray facilities. These fields were deemed to be representative of the broader areas of research. While only selected areas were examined, the results for these subfields were all qualitatively similar, suggesting that the findings articulated below are representative of research of interest to DOE's Office of Basic Energy Sciences.

An assessment of impactful scientific publications and expert analysis of recent conference data was used to gauge leadership in the chosen fields. The impact of scientific publications was evaluated based on citation count and parsed by geographical region and country of origin of the corresponding author. The data were collected over three decades (1990-2020). Details of the methodology and analysis are described in detail in the Appendix. The scientific impact of major user facilities was assessed by analyzing the use of specific facilities in the most highly cited papers integrated over the entire 30-year period. Due to the relatively small numbers of high-impact publications, the cross-cutting analysis could not be performed for smaller time increments. Conference data were analyzed using a modification of the methodology suggested by a previous report.[3] The conference data were in qualitative agreement with citation data for a decade earlier; i.e. conferences in 2019 reflected the citation demographics in 2010 or earlier. This reflects the tendency that it takes some time for the work to be broadly recognized and the researchers being invited to present in conferences. The conference data are also less systematic. Therefore, these data are summarized in the appendix only. In both the citation and conference analysis, we saw evidence of "home field advantage" in that the papers in a certain geographic region tend to cite work in that region more, and conferences tend to have more representation in the region where the conferences were held. However, these factors are unlikely to account for the major time dependent trends uncovered in this study, as such "home field advantage" would present itself in all times.

Description of the Fields

The fields identified for detailed analysis were all deemed essential to the Department of Energy's basic energy sciences mission. These are all fundamental areas of research that will potentially contribute to new technologies and applications. Fundamental research funded by DOE Office of Basic Energy Sciences has made significant impact on the U.S. economy with many benefits to society, as summarized in a 2018 BESAC report.[4] Brief descriptions of the areas studied and their potential applications follow below.

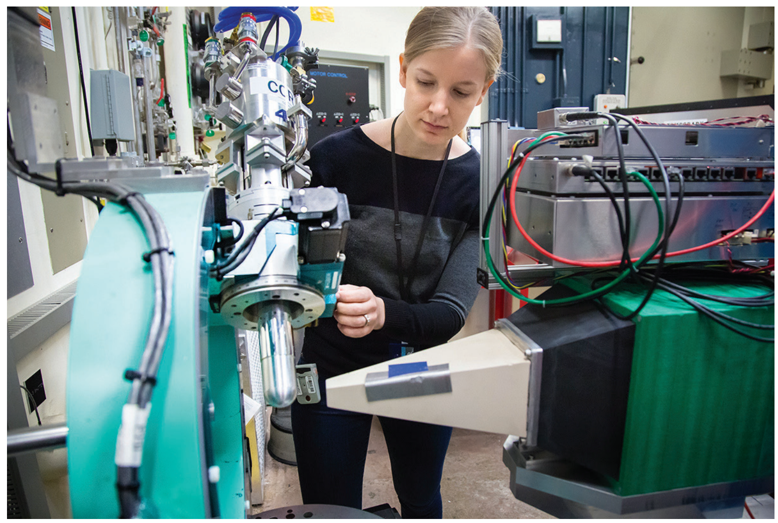
Quantum information science

Quantum information science emerged from the intersection of quantum physics and information science. The field has grown enormously since the demonstrations of exponential quantum speedup for quantum algorithms and the possibility of fault tolerant quantum computation. Today the field includes quantum computation, quantum communication, quantum simulation, and quantum sensing.

3. Committee on Science Engineering and Public Policy, *Experiments in International Benchmarking of U.S. Research Fields* (Washington, D.C.: National Academies Press, 2000), www.doi.org/10.17226/9784

4. "A Remarkable Return on Investment in Fundamental Research. 40 Years of Basic Energy Sciences at the Department of Energy" (U.S. Department of Energy, Office of Science, 2018), www.science.osti.gov/-/media/bes/pdf/BESat40/BES_at_40.pdf

In each of these areas there has been significant and accelerating progress in experimental implementation of quantum protocols. In particular, quantum computation and quantum simulation have both already reached the point where experiments on near term quantum devices are challenging the limits of their classical counterparts, with claims of 'quantum supremacy' in both areas. Quantum communication that is ensured to be secure because of the principles of quantum mechanics has already been implemented with earth to satellite links integrated into large scale terrestrial networks, promising secure distributed quantum networking. (See Box 1.1. A Testbed for Secure Quantum Communications.) Each of the four pillars of quantum information science today have many scientific applications within the BES domain. Methodological developments underway in quantum computation and quantum simulation will significantly expand our capabilities to understand and control the dynamics of non-equilibrium systems. This includes the key area of predicting the energetics and dynamics of strongly correlated electronic systems, an important task for understanding chemical reactions and catalytic behavior, as well as for enzymatic and photosynthetic systems in biology. Significant effort is also being invested in development of quantum algorithms for computation and simulation of materials, enabling fundamental studies of condensed phase systems beyond the capabilities of classical computers. Exploitation of quantum concepts such as entanglement and squeezing can yield significant improvement in precision measurements. Substantial advances in quantum technologies have already led to quantum-limited vibrational sensors and accelerometers, while networks of quantum clocks, i.e., quantum GPS, can function as highly accurate gravitometers to probe seismic faults. Novel materials have been developed for quantum sensing, such as nitrogen vacancy defects in diamond and other defect systems that can operate as quantum limited magnetometers, electrometers, and thermometers for direct imaging of a broad range of physical, chemical and biological systems. Quantum photonic technologies are also new opportunities for imaging and for biophotonics, with the ability to study photo-initiated processes in biological systems with quantum light sources. In addition to this broad range of applications in BES related science, quantum computation and quantum communication also have significant applications in the financial, business, and economic ecosystems.



University of Tennessee-Knoxville researcher Paige Kelley uses the Oak Ridge National Laboratory High Flux Isotope Reactor to study materials critical to quantum computing. (CREDIT: GENEVIEVE MARTIN/ORNL)

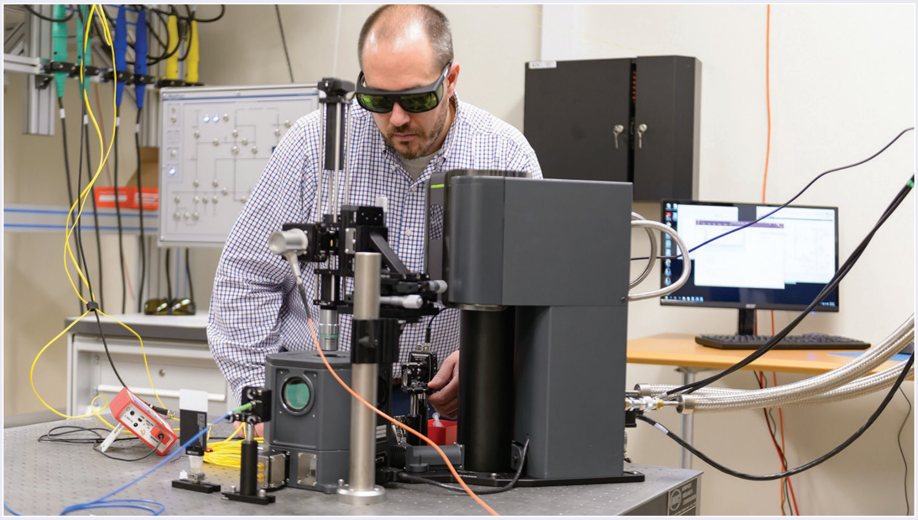
Science for energy applications—Energy storage

The field of energy storage encompasses the variety of technologies that enable energy to be stored at one time and used later, and is necessitated by the imbalance in the times and rates of energy production and demand. Electrical energy storage in batteries and related devices is critical for integrating renewable energy sources such as solar and wind power into the electrical grid, as well as for transportation, internet and computing, domestic security, and personal electronics. Fundamentally broad and interdisciplinary in character, research on electrical

BOX 1.1. **A TESTBED FOR SECURE QUANTUM COMMUNICATIONS**

Turning the spooky phenomenon of quantum entanglement into an unhackable next-generation internet

Stealing information by hacking into computers and internet systems happens everywhere. Even sensitive federal government systems are not immune. Moreover, the next generation of quantum computers will be able to overcome today's encryption techniques, rendering them largely useless. Quantum communication systems could not only secure data transmissions, but will also enable links between quantum computers to create quantum supercomputers. That accounts for the intense national security interest in quantum communications, and explains why the U.S. Department of Energy's Office of Basic Energy Sciences is supporting both fundamental research and testbeds, such as the effort at Argonne National Laboratory near Chicago. There are also vigorous efforts in Europe, Japan, and especially China, which just announced an important milestone in related research.



Argonne scientist Alan Dibos aligns optics to study materials for a possible quantum repeater device; the materials are in a cryostat that that keeps them at a temperature just 3 degrees above absolute zero.
(CREDIT: ARGONNE NATIONAL LABORATORY)

Quantum entanglement means that two or more particles—such as photons—are inextricably linked: if the quantum state of one changes, so does the quantum state of the other, instantaneously. The spooky part is that this linkage is *not* dependent on distance; it works whether the particles are close together or many miles apart. In addition, the act of reading the particle modifies its quantum state. So, a communication system that transmits one of each pair over optical fibers could securely carry information, because any attempt to intercept and read that data would be unambiguously detected.

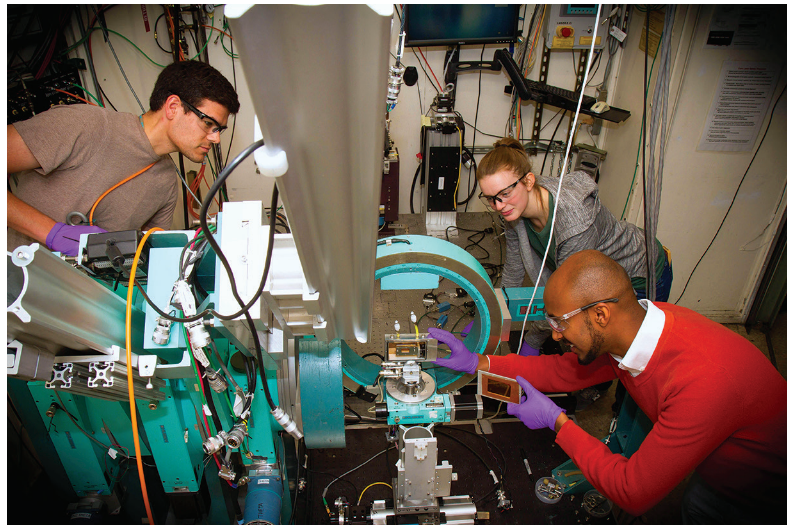
Today, optical fibers already carry nearly all long-distance data transmissions, with wireless links operating only between our mobile devices and the nearest communications tower. Because the signal strength of the light beam in a fiber gradually weakens, optical fiber networks have repeater stations about every 40 miles, even underneath the oceans, that read and retransmit the data. This is the backbone of today's internet. And since a light beam consists of a stream of photons, using entangled photons could in principle secure the data transmission. In practice, however, the repeaters for quantum communications remain to be developed and pose a significant challenge for both fundamental science as well as practical technology: quantum states cannot simply be read and retransmitted.

That's what the Argonne National Laboratory testbed is working on. The testbed consists of two connected 26-mile loops of fiber optic cables that can transmit entangled photons. The research focuses both on better understanding the quantum behavior of paired photons and on developing and testing potential quantum repeaters. The laboratory is partnering with both the University of Chicago and several startup technology companies—creating what is essentially an innovation ecosystem to accelerate progress. The testbed network is currently being extended to the University of Chicago and to downtown Chicago to create a U.S.-based metropolitan-scale network.

One potential repeater system under investigation at Argonne would store the quantum state information from each transmitted photon in the spin state of a defect within a solid state material—the analogue of isolated atoms in matter—then export it to a new photon for the next leg of the journey along an optical fiber. The storage and re-transmission takes place in less than 100 milliseconds. A stream of such entangled photons and their quantum states would be analogous to the string of 1's and 0's in a conventional computer or internet data stream. Since quantum entanglement has no classical analogue, however, there remain many fundamental questions: What triggers loss of entanglement? What repeater design is most reliable? How best to design and integrate single photon detectors to read the information?

David Awschalom, who oversees the Argonne quantum communications testbed, says that no research groups have yet fully answered these questions—that the relevant science and technology are only now emerging from fundamental research and thus can benefit from open collaboration. At the same time, he acknowledges the stakes involved for national competitiveness. A team at the University of Science and Technology in China, for example, recently published results showing that they had successfully entangled two quantum memories—rubidium atoms chilled to extremely low temperatures—at a distance of 31 miles, a step towards a possible quantum repeater. So the pressure is on, and prize is the ability to build a unhackable quantum internet, which would be of immense national security and commercial value.

energy storage lies at the crossroads of electrochemistry, chemistry, and materials science. While past advances have been transformational, for instance leading to the Li-ion battery that has revolutionized personal electronics, substantial ongoing research focuses on improvements in the current technology. Goals include an increase in the lifetime, efficiency, safety, and recharging speed of current battery types, and the advancement of the fundamental understanding of chemical transformations related to battery performance. Examples of areas of scientific study include the migration of electrons, atoms, and ions through materials in harsh conditions, study of new electrochemical transformations, focus on characterization and understanding of complex dynamic interfaces, and discovery of new materials for battery components: anodes, electrolytes, and membranes. This new fundamental understanding will enable profound advances for future electrical energy storage technologies, for instance with greater energy density, efficiency, reliability, and sustainability, expanding the horizons of mankind for improved quality of life, and access to unforeseen goals, for instance space travel.



Stanford University graduate students install an X-ray cell for battery research using the SLAC National Accelerator Laboratory X-ray synchrotron.
(CREDIT: JEN HOSTETLER/SLAC)

Science for energy applications—Membranes

The ability to selectively separate different chemical species is an internal function critical to the operations of diverse energy technologies. A variety of different membranes are therefore required to enable processes and devices for energy production, harvesting, and storage. For instance, the development of specialized polymer membranes allowing the selective transport of protons has enabled hydrogen fuel cells, a clean technology holding the potential, with its rapid refueling capacity, to revolutionize transportation and power generation. Polymer membranes are also critical to the operation of liquid electrolyte batteries, separating the anode and cathode to prevent a short circuit while allowing select ions to pass. Metal organic framework membranes are critical to gas purification for energy and other applications. Of particular importance, many energy technologies from petroleum to hydroelectric power are water-intensive while, at the same time, water itself is scarce in much of the world, critical to agriculture and the sustaining of populated regions, and requires large amounts of energy to purify and desalinate. Therefore energy production and water purification are overlapping and integrated, with membranes playing a key role to remove particles, chemicals, organisms, and ions. Research in membranes focuses on the fundamentals of diffusion in confined spaces, development and synthesis of new polymers that are able to withstand the harsh conditions in batteries and fuel cells; material compositions with selective affinities for ions and targeted species; surfaces with anti-fouling properties; and materials morphologies with tight control of pore sizes and robust mechanical properties to withstand high operating pressures. Research also targets new membrane materials for next generation applications, especially those with integrated multiple functionalities such as catalytic activity, biomimetic reconfigurability, and integrated active and selective transport mechanisms beyond basic diffusion. These advanced membranes for energy and water will remain critical to sustaining populations in the growing regions where water is becoming increasingly scarce; at the same time membranes will play a leading role in revolutionizing transportation and electricity supply that will enable renewable energy technologies.

Matter for energy and information—Quantum materials

The electronics industry rests on the control of the properties of electrons inside materials. Since the invention of the transistor, the most important material has been silicon. Amazingly, the phenomenal progress of Moore's law (the doubling of the number of transistors on a chip about every 18 months) has been achieved mostly by treating the electrons in silicon as classical particles. However, Moore's law is now breaking down and the reduction of the size of transistors has leveled off. What will advance technology in the future is uncertain, but will likely involve materials other than silicon—materials in which quantum mechanics plays a much more central role. For example, superconductivity, the complete loss of resistance below some critical temperature, is a macroscopic manifestation of quantum mechanics. While this phenomenon has been known for 110 years, the discovery in 1986 of a class of materials with critical temperatures that are above that of liquid nitrogen has made superconductors useful in electronics as well as in transporting power over long distances without loss. There is still no universally accepted theory of this phenomenon and new materials are discovered every few years that help improve understanding of this phenomenon. About 15 years ago another class of materials—called topological insulators—was predicted and then synthesized. These materials are insulating in their interiors but have metallic surfaces on which electrons in principle could move with no resistance. Theory suggests ways in which such surface electrons could be used to form the building blocks of quantum computing; they may also be useful for quantum sensing. Most recently, there has been great excitement because of a discovery in the properties of layers of carbon a single atom in thickness, a material known as graphene. When two such layers are stacked with a special twist angle between them, a wide variety of new phenomena appear including superconductivity. In effect, this gives scientists the ability to control the quantum behavior of electrons in graphene by mechanically varying the angle between two atomically thin layers, which opens up enormous possibilities for science and technology. Such discoveries of new classes of electronic materials or new ways on controlling the properties of electrons within materials every decade or so makes the field of quantum materials one in which the U.S. must remain competitive.

Industrially relevant science—Polymer upcycling

With the numerous advances of macromolecular chemistry, natural resources such as coal and oil and the byproducts of their extraction have been readily converted into polymers to make a plethora of products. Currently, only a small fraction of the hundreds of million tons of polymers that are produced each year is recycled, which is unsustainable and undesirable. Polymeric materials are generally quite durable, which leads to their widespread use but which also poses problems for recycling. The most economical way to recycle polymers is through melt-reprocessing, in which polymers are heated to a high enough temperature to be shaped and molded into new shapes and products. However, melt-reprocessing tends to degrade the polymer, reducing its quality, and is costly. Additionally, polymer networks where polymer chains are sufficiently cross-linked cannot be recycled in such a manner. The goal for the field of polymer upcycling is to dramatically reduce the need to manufacture new polymer materials by making it cheaper and easier to use upcycled materials to manufacture higher-value products rather than extracting and using new resources. It is a multi-faceted challenge which extends across multiple scientific disciplines. Several scientific advances in chemical catalysis, interfacial phenomena and polymer science are anticipated. (See Box 1.2, Creating the Chemistry for Better, Smarter Materials.) Chemical and physical methods to modify polymer surface properties to promote catalysis, such as the synthesis of polymeric compatibilizers that promote catalyst adhesions to other polymer surfaces and enhance catalytic action, will be pursued. The development of new polymer chemistries can also lead to new and more sustainable materials. The usage of non-covalent bonds between constituent monomers, for example, may provide novel methods to upcycling polymers. Dynamic covalent bonds, which may break and reform in response to various stimuli such as light or heat, may enable alternate methods to recycle networks. Technological advances aiming to break down polymers into their monomer constituents to be readily remade into new polymers are also anticipated.

Industrially relevant science—Electrochemical energy conversion

The interconversion of electricity and energy is central to sustainability in the economy. For example, energy storage, discussed above, relies on storage of electrical energy for future use. Conversion of fuels to electrical energy for use on the grid is another example. Removal of CO_2 from the atmosphere and conversion to useful products is another critical application. Fundamental studies of electrochemistry are currently addressing challenges in the field that will provide the basis for new approaches to these important applications. The fundamental challenges range from understanding the chemical processes to

BOX 1.2. CREATING THE CHEMISTRY FOR BETTER, SMARTER MATERIALS

Fixing plastic pollution, self-regulating polymers

Some of the most common and useful materials are polymers—large molecules composed of repeating units. Naturally occurring biological polymers include hair, cellulose in wood, and even the DNA that carries the genetic codes for all living things. Synthetic (human-made) polymers include nylon and other plastics, where the repeating units are most typically carbon and hydrogen made from petroleum or natural gas. Some newer polymers can even respond to environmental changes, just like many biological materials, and can be used to create "smart" materials.

Plastics, however, are ubiquitous. Globally we produce some 400 million tons per year for packaging, consumer and industrial products, and many other applications. About 40 percent of that is for single use packaging that is promptly discarded, creating a lot of landfill waste, uncollected plastic litter, or ultimately plastic pollution in the oceans that can last for centuries. The problem is that many current plastics cannot be recycled and reused, so there is no incentive to gather and sort them. Indeed, less than 10% of U.S. plastic waste is recycled, creating a real and growing problem.

Because waste plastic is not perceived as valuable, there is no incentive to gather and sort it, absent government mandates (generally lacking in developing countries). Sorting is important, because the polymers in the six major types of plastics cannot be physically mixed. That is especially true for polyethylene and polypropylene, which together account for more than half of all plastics produced: if melted together, they make a brittle material of little practical use.

One approach being undertaken by a research team from five universities and two DOE national laboratories, coordinated by Aaron Sadow of Ames Laboratory and Iowa State University, is to look for low-hanging fruit by adapting chemical processes for conversions of plastics. The team is developing several new catalysts that can break up polyethylene's carbon-carbon bonds, potentially creating precursors to lubricating oil, cleaners and soaps, cosmetics, even cooking oil. The intent is to create products that have commercial value, which both reuses waste polyethylene and creates an incentive to gather such waste.

Another approach is to find a way to bond polyethylene and polypropylene together to create a new material that had some of the properties of both—in effect, upcycling (upgrading as well as recycling) the material. Geoffrey Coates and Anne LaPointe of Cornell University along with Frank Bates of the University of Minnesota and their research teams designed a catalyst that makes a binding material—called a multiblock co-polymer—that links recycled polyethylene and polypropylene together to make a tough composite. After nearly five years of work, the system can create useful products from the recycled plastics using extremely small amounts of the binding material. Moreover, the unique properties of the composite mean that, for many applications, smaller quantities of plastic are needed. Coates has formed a company, Intermix Performance Materials, to scale the process toward industrial use. Potentially, this process could stimulate increased recycling while reducing use of the fossil fuels from which nearly all plastics are made.

continued on page 14

continued from page 13

Longer term, the world needs something better than today's plastics. A team at DOE's Lawrence Berkeley National Laboratory is working to create new kinds of plastic materials that are designed for re-use and thus can enable a more closed material cycle. What motivates this approach are rapidly evolving new methods of manufacturing, driven by advances in digital manufacturing—analogous to 3D printing or additive manufacturing. Digital manufacturing makes possible the use of novel materials and new ways of forming the molecular bonds that hold these materials together—and thus potentially capable of easy disassembly, because strong acids can uncouple their molecular bonds. More research is needed to understand how to control the nanoscale processes involved in using such materials in digital manufacturing. But as manufacturing itself evolves into a smaller scale, more distributed activity, so might the materials that it uses evolve—in ways that are designed for multiple re-use with much reduced environmental impact.

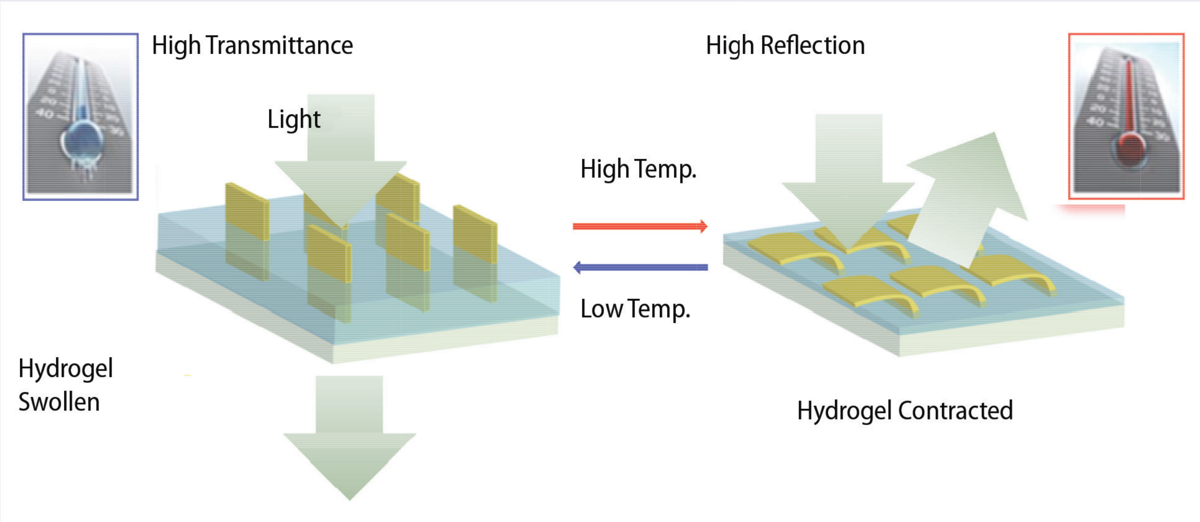
Truly smart materials that can adapt to changing environmental conditions, however, need a very different kind of polymer—one that can alter its properties. For example, polymers called hydrogels can absorb water, and when that happens, the polymer expands, creating a kind of synthetic muscle that can be used to drive physical changes. Hydrogels can also respond to changes in temperature, acidity, electric fields or even light, depending on their composition. That means these materials can, in effect, use energy from their environment (such as sunlight or rising temperature) to cause a chemical change in the hydrogel polymer, which in turn could regulate the material's optical, thermal, mechanical or transport properties.

Joanna Aizenberg in her laboratory at Harvard University (CREDIT: JOANNA AIZENBERG)

It is the potential for such self-regulating systems that excite Joanna Aizenberg, a Harvard chemist who has been working on these materials with DOE support for nearly a decade. Because hydrogels can respond to environmental changes across a wide range of conditions and can be combined with other types of materials to form hybrid systems, Aizenberg believes that these materials will have many uses. She points to four broad types of applications, among many opportunities that lie ahead:

- Synthetic hydrogel muscles that actuate nanostructure "bones" to power autonomous systems such as robotic devices capable of capturing impurities and particulate matter, inducing movement and propulsion, or regulating chemical reactions, based on environmental changes;
- Medical applications, such as polymer substrates to guide wound-healing, cell differentiation and tissue growth in a particular shape or orientation;
- Smart windows coated with a temperature-responsive hydrogel muscle that puts in motion embedded reflective nanostructures, thus self-adjusting the window's transparency and reflecting excessive heat in response to rising temperatures (see illustration);
- Antennae that turn toward a light source, enabling solar panels to stay focused on the sun as it moves across the sky for optimum power generation.

Taken together, these research efforts to push polymer chemistry into new territory promise not only to alter familiar plastics in ways that solve a serious pollution problem, but also to create genuinely smart materials for a myriad of practical applications. In effect, synthetic polymers are becoming more akin to biological materials in their ability to adapt to environmental conditions and self-optimize and, like the tissues in our bodies, to be recycled and reused.



Schematic showing the mechanism by which temperature-sensitive hydrogel polymers can self-regulate the transparency of window
(CREDIT:DR. PHILSEOK KIM, AIZENBERG LAB)

creation of new materials. The work in this area will enable new approaches to electrification of transportation, sustainable production of chemicals and products used for everyday life, and harnessing the energy of sunlight for useful purposes.

Results

In all cases studied, the analysis of the top 20% of cited literature clearly showed that the U.S. is losing ground to foreign competitors and, in some cases, is already lagging behind (see Figure 1 on page 16). The U.S.'s relative position improves when analyzing top 5% cited literature (see Appendix), but qualitative trend remains similar. In the emerging area of Quantum Information Science, for example, the EU is clearly leading, with China and the U.S. close behind. In other areas studied China is emerging as a worldwide leader. The changes in leadership in these areas correspond to a period of rapid increase in research investment in China and a flattening in the research funding in the U.S., suggesting that investment in key areas has a significant impact on leadership.

The leading publications as of 2019 were led by authors from China in the areas of membranes, energy storage, and sustainable energy science (electrocatalysis and polymer upcycling). For example, nearly 60% of the top papers cited in 2019 in all of these areas were led by authors from China (see Figure 1 and Appendix). China's leading position developed rapidly; for example, in the membranes area, Chinese publications accounted for ~10% of the top publications in 2010 rising to ~60% in 2019. At the same time, the U.S. and EU positions diminished, dropping from ~40% and 20%, respectively, in 2010 to ~10% in 2019. The U.S. is likewise losing ground in sustainable energy development, including electrocatalysis, electrochemical energy storage and polymer upcycling (see Appendix); and is clearly lagging behind in the critical area of energy storage (see Figure 1, top).

The U.S. has maintained a solid position in the area of quantum information science, although the EU is leading and China has overtaken the U.S. (see Figure 1, middle). Overall, the EU and U.S. position is relatively flat since 2010 accounting for ~40% and ~20% of the top cited papers. In comparison, China has surpassed the U.S. in 2019 after producing only ~10% of the top papers in 2010.

The U.S., EU, and China are all contributing similarly as of 2019 with somewhat less than 30% of the share of the highly-cited papers in the field of quantum materials (see Appendix). Again, the impact of research from China is rapidly emerging in this area. The U.S. position has diminished over time, reaching the lowest point in 2019 in the 3-decade period studied. In the 1990s, the U.S. was clearly leading producing around 50% of the important papers, but that share fell until the early 2000s followed by another period of growth until ~2010. In the area of quantum materials, U.S., EU and China are on par with each other, with China improving from a distant 3rd to its current position.

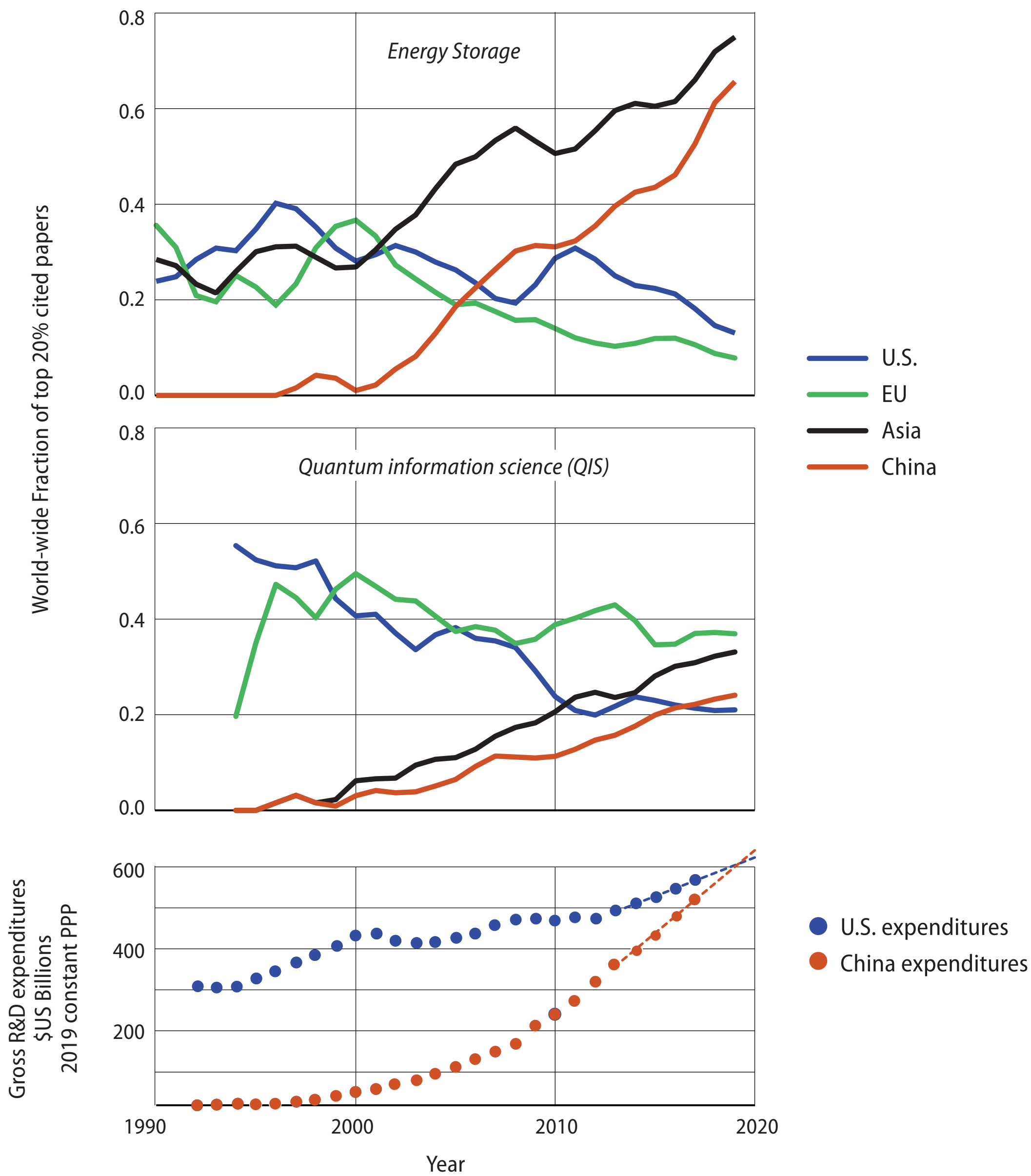


FIGURE 1. Selected literature search results. For each year, the fraction of top-20%-cited papers published by authors based in the U.S., EU, Asia (including China) and China are shown for the topics Energy Storage (top) and Quantum Information Science (middle). The markers are the raw data from each country or region, the solid lines present smoothed data so the trends are easier to follow. Gross R&D expenditures (in $US Billions at 2019 constant PPP) for U.S. and China (adapted with permission*) are shown for comparison (bottom), the dots represent actual expenditures, the dashed lines are a linear extrapolation.

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* *The Perils of Complacency, America at a Tipping Point in Science and Engineering* (American Academy of Arts and Sciences, 2020), www.amacad.org/publication/perils-of-complacency

2. ADVANCED RESEARCH TOOLS

Large-scale research facilities are important investments that have very significant scientific impact. The use of key DOE Basic Energy Sciences facilities has resulted in numerous scientific breakthroughs, signified by recognition through major awards including multiple Nobel Prizes. This section of the report focuses on very large-scale facilities: X-ray synchrotrons; X-ray free electron lasers; and reactor-based and spallation neutron sources.

Analysis of the use of these facilities in the most highly-cited papers showed that use of the facilities varies by subfield and that geographical proximity is a major determinant of facilities use (see Appendix). Generally, researchers use facilities in their home countries or world region; in other words, U.S. researchers most heavily use U.S. facilities, EU researchers mainly use facilities in the EU, and so on. Nevertheless, the preeminence of U.S. facilities for specific areas of research, such as quantum materials, is reflected by their wider use by researchers from around the world.

X-ray synchrotrons have expanded rapidly, with experimental stations at such facilities doubling globally over the past 20 years to more than 875, while the number of U.S. experimental stations at such facilities has remained roughly constant at 186. The result is significant U.S. capacity constraints that limit research progress and make foreign facilities more attractive. Current U.S. synchrotron upgrades will temporarily restore technical leadership as measured by source "brightness," but only until completion of other new foreign facilities.

The U.S. built the world's first X-ray free electron laser facility, and is now expanding and upgrading that facility, ensuring at least near-term technical leadership. But EU is also upgrading its X-ray laser facilities and expanding its experimental stations; China is constructing a facility that will provide similar technical quality to the U.S. but with more experimental stations (and user capacity).

The U.S. also risks falling behind in spallation neutron sources due to new European facilities and expanded experimental stations. And due to the need to upgrade or replace the U.S. high flux reactor neutron source—important for basic research and at present the only facility for production of certain radioactive isotopes critical for medical and national security applications—that leadership is also at risk.

X-ray Sources

Ultra-bright X-ray sources—synchrotron storage rings and free electron lasers—are powerful scientific tools that give researchers the ability to probe deeply into materials down to the molecular and atomic levels and to observe reactions that take place within a nanosecond. Using these extraordinary capabilities, scientists and engineers have created next-generation battery materials, developed life-saving drugs, fabricated stronger building materials, and transformed information systems (See Box 2.1. Building a Better Battery for Clean Energy Storage, and Box 2.2. Transforming Structural Biological Science).

The scientific advances made possible by these powerful machines have driven huge economic benefits, leading to intense global competition for access to the latest machines with the greatest capabilities. As we look to the future, the United States' scientific and economic leadership will require ongoing investments in leading-edge facilities that will attract world-class researchers and support exceptional scientific inquiry across multiple disciplines.

BOX 2.1. **BUILDING A BETTER BATTERY FOR CLEAN ENERGY STORAGE**

How fundamental research coupled with an emerging U.S. innovation ecosystem created a novel energy storage system

The lithium-ion battery that powers all our mobile devices and, increasingly, electric vehicles, was first proposed by a U.S. scientist, who later shared a Nobel Prize. The lithium battery manufacturing industry, however, has largely been captured by Asian companies.

Energy storage will also be critical for renewable energy sources such as solar and wind power to power the electrical grid and for many other non-mobile applications such as data centers and telecom towers. These applications need energy storage solutions that charge and discharge rapidly, don't wear out in a few years or a few thousand charge-discharge cycles, and are made from less expensive materials than lithium-ion batteries. Just such an energy storage technology—a sodium-ion battery—is now being produced by a U.S. start-up company, and may offer the U.S. a new chance at competitive advantage. How this innovation came about is instructive.

When Colin Wessels was a graduate student in materials science and engineering at Stanford University, his advisor, Bob Huggins, had an intriguing idea. Smart windows that turn partially opaque when the sun is too bright are coated with a material that changes color by transferring electrical charge from one part of the material to another. Could that same phenomenon be used to store energy and hence to make a battery as well? Colin set out to test the idea. After a number of trials, he settled on a sponge-like material called Prussian blue, a synthetic pigment long used by artists for its vibrant color as well as in glass-making and a variety of other industrial applications. From Colin's perspective, the key characteristic of the material was its crystal structure—a lattice anchored by either iron or manganese atoms bonded to carbon and nitrogen atoms with lots of interior spaces that enable it to accommodate and store sodium ions. That enables rapid movement of sodium ions into and out of battery electrodes made from the material, transferring electrical charge as the battery discharged, and back again during recharging—just as lithium ions do in today's batteries. He built his initial batteries using an iron-based cathode material.

Colin Wessels, founder and CEO of Natron Energy

The prototype battery seemed to work, but a challenging issue was to find a suitable anode material. In mid-2012, Colin founded a company, persuaded the Molecular Foundry at the Department of Energy's Lawrence Berkeley National Laboratory to provide laboratory access to develop Prussian blue anode materials, and moved into a friend's garage in Palo Alto (since he had no income or funding). The Foundry helps researchers synthesize materials and fabricate them into testing devices. With their assistance (and a year of hard work), Colin found a compatible and low-cost anode material based on the manganese form of Prussian blue. But a larger—potentially fundamental—problem emerged: the manganese atoms in this electrode appeared to show a state of charge that chemists believed impossible. No one could explain how the battery worked well, or why it worked at all. If the working mechanism was unclear, so was the reliability of the technology for the proposed battery, which meant that the fledgling company would have trouble attracting investment.

While struggling to understand what was going on in his battery, Colin happened to meet Wanli Yang, a physicist at the Advanced Light Source (ALS) X-ray synchrotron. The ALS is another division of the Berkeley Laboratory, which uses X-ray spectroscopy to probe material properties at the elemental level. Intrigued with a fundamental science mystery, Wanli agreed to collaborate with Colin. He and his team used an advanced spectroscopic method developed at the ALS to study the manganese electrode. They made the remarkable discovery that the manganese atoms in the Prussian blue material were indeed in a novel chemical state, ideal for a battery anode. Moreover, they found that the cycling of the battery triggers chemical reactions involving a physical property of electron spin states, which largely determines the battery operation voltage. The scientists published papers about the unique chemistry and fundamental physics they had discovered; Colin raised money and set about building a company.

That company—Natron Energy—is now scaling up its manufacture of the batteries, which use both iron and manganese forms of Prussian blue in their electrodes. The novel batteries are finding a ready market. Indeed, mobile applications aside, sodium ion batteries appear to have major potential advantages over lithium ion batteries:

- Chemical reactions between lithium ions and the electrodes in those batteries eventually degrade their performance, but there are no such reactions in sodium ion batteries, which means a far longer lifetime (and hence a lower cost for energy storage).
- The battery can charge or discharge very quickly, in a few minutes, which helps data centers, hospitals, telecom towers, and other critical facilities meet sudden surges in computing needs or sudden power outages.
- The raw materials for the battery are also less expensive than those for lithium ion batteries—sodium, manganese, and iron are among the most plentiful elements on earth—which means that as production scales up and costs come down, these batteries could potentially contribute to grid-scale energy storage that expanded use of renewable energy sources such as solar and wind will require.

Companies in Asia and the U.K. are also developing sodium ion batteries and there are other novel storage technologies under development, but at least a U.S. company now has the potential for a competitive edge. Moreover, the productive interaction between the DOE national laboratory and California's university/entrepreneur-based innovation ecosystem continues to expand, fostering still more innovations. Indeed, Colin's experience was one of several that helped stimulate the creation of an enterprise accelerator—Cyclotron Road—to support similar energy start-up companies.

(Top) The chemical reactor set-up Colin Wessels used at the Molecular Foundry for making Prussian blue materials, with a synthesis in progress (CREDIT: NATRON ENERGY)

(Bottom) The inside of the vacuum chamber at Lawrence Berkeley National Laboratory's X-ray synchrotron that was used to study and resolve the novel chemical state of the manganese atoms in the Prussian blue battery electrode (CREDIT: WANLI YANG)

X-ray Free Electron Lasers

The United States has led the world in the field of X-ray Free Electron Lasers (XFELs) since the 2009 delivery of the world's first hard X-ray facility, the Linac Coherent Light Source at the SLAC National Accelerator Laboratory (see Box 3.4. Why Long-Range Planning Is Critical To U.S. Competitiveness). The facility is now being expanded and upgraded with realization of LCLS-II and LCLS-II-HE, which will be the world's first continuous wave X-ray sources spanning both soft and hard X-ray ranges. These improvements, which will provide fully coherent ultrafast X-rays in a continuous, programmable pulse structure up to MHz rates, represent a leap of four orders of magnitude as compared to LCLS, and will maintain U.S. technological primacy in the near term.

Over the past decade, however, governments in Europe and Asia have built a number of new XFEL facilities with capabilities that currently surpass LCLS in some respects, and next-generation upgrades and new facilities are now under construction.

At present, the European XFEL's average brightness is more than 100 times greater than other operating XFELs, although the pulse structure (10 Hz delivery of 4.5 MHz bursts) presents significant technical and scientific limitations. The facility has announced plans to build a second fan of beamlines (experimental stations), as well as a new experimental hall supporting specialized instruments with more than three times the capacity of LCLS. A subsequent upgrade will enable continuous MHz operation. (A comparison of current and proposed capabilities for these facilities is shown in Figure 2, with "average brightness" as a figure of merit for measurement sensitivity/fidelity and ability to probe at the extremes of time and spatial resolution.)

China is now three years into the construction of the SHINE XFEL facility, which is intended to match or exceed the capabilities of LCLS-II-HE. SHINE will be equipped with 75 cryomodules, versus 55 for LCLS-II-HE, which will feed a set of superconduct-

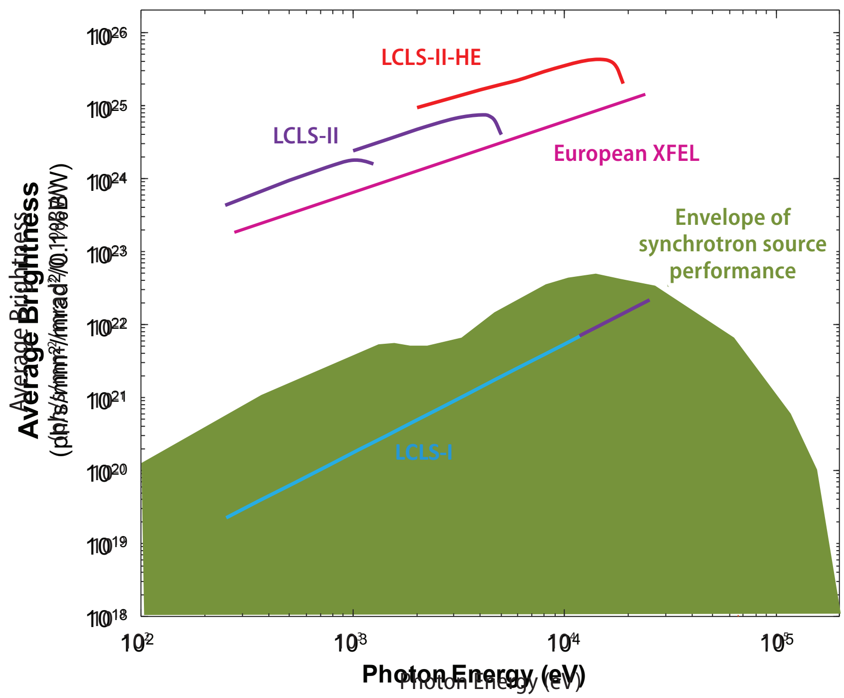


FIGURE 2. Comparative plot of the average brightness of the LCLS facility, along with representative curves for the European XFEL and synchrotron sources. Other current XFEL sources are comparable to LCLS-I; SHINE will be at the level of LCLS-II-HE or higher.

ing undulators and three independent beamlines and will likely allow a higher electron energy reach.

The United States also has been far outstripped in terms of the number of beamlines and instruments it hosts. The four XFEL facilities in Europe (Eu-XFEL, SwissFEL, FERMI and FLASH) and three in Asia (SACLA, PAL-FEL and SXFEL), represent a total of 16 independent beamline sources and 36 independent instruments, as compared with two U.S. beamlines and eight instruments. The United States is expected to fall even further behind in terms of beamline and instrument capacity over the next decade, as shown in Figure 3.

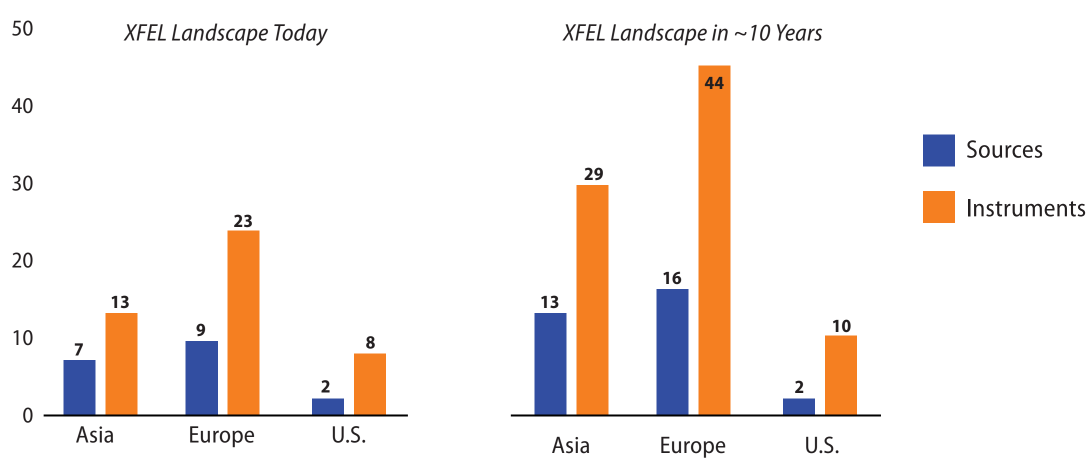


FIGURE 3. Comparing numbers of independent XFEL sources (i.e., undulator beamlines) and instruments (i.e., physically separate, independent experimental stations) in the U.S., Asia, and Europe today vs. 10 years from now, based on announced projects

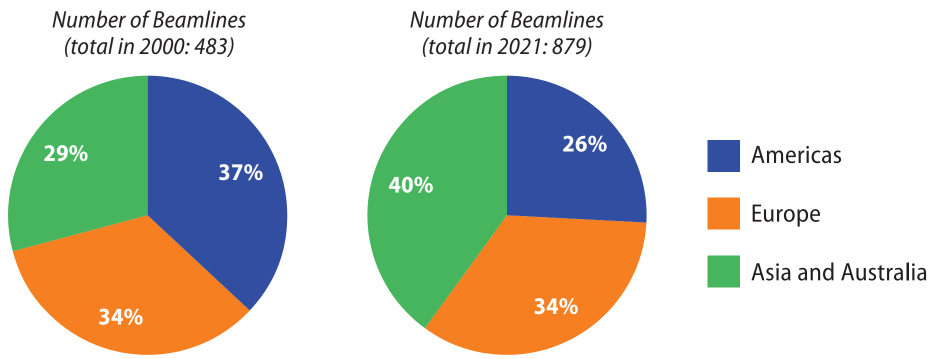


FIGURE 4. Number of synchrotron beamlines by geographical area. In 2000, there was a total of 483 beamlines in the world, in 2021 there are 879.

Synchrotron Sources

Over the past 20 years, the United States has been rapidly outpaced in the number of beamlines (i.e., experimental capabilities) provided at world-class synchrotron sources. In 2000, there were 483 beamlines worldwide; 170 of them were in the United States. Today, the total number of beamlines in the world has nearly doubled, to 879, while the number of U.S. beamlines has remained roughly constant at 186. By comparison, the number of beamlines in China has doubled in this period.

The United States also has been challenged in terms of facility performance, as measured by source brightness. Revolutionary technological improvements have enabled enormous gains in brightness at synchrotron sources overseas, and the United States has fallen behind. Although the ongoing APS-Upgrade and ALS-Upgrade projects will restore U.S. leadership in source brightness, China's HEPS is likely to take world-leadership in brightness, as shown in Figure 5. Significant, continuing upgrades will be required to reinforce U.S. competitiveness in the coming decades.

Researchers work on analyzing X-ray fluorescence images of samples produced with the Brookhaven National Laboratory's X-ray synchrotron.
(CREDIT: BROOKHAVEN NATIONAL LABORATORY)

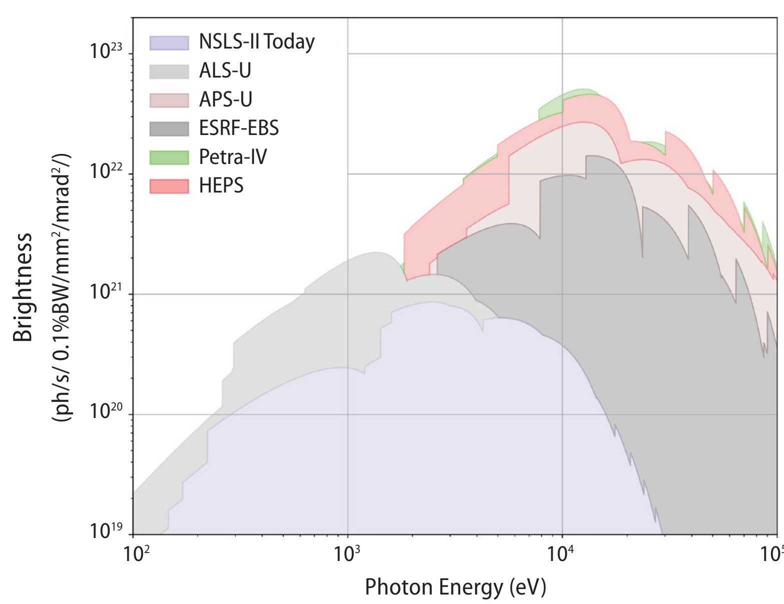


FIGURE 5. Brightness of U.S. synchrotron sources NSLS-II, ALS-U and APS-U compared with ESRF-EBS (France), Petra-IV (Germany) and HEPS (China)

BOX 2.2. TRANSFORMING STRUCTURAL BIOLOGICAL SCIENCE AND BIOMEDICINE

How X-ray sources enabled an understanding of the molecular machines that power life

Proteins are an important part of our diet because they contain amino acids that our bodies need but can't synthesize. Proteins also provide much of the structure of our cells and play a critical role in how our bodies function, for example as enzymes and antibodies. In addition, proteins are an essential part of larger molecular machines, such as those which create new proteins within cells. In fact, proteins are the most common and also the most diverse molecules in all living things.

Yet much of what we know about proteins—and especially about their molecular structure—has been discovered only in the past 25 years using advanced research facilities. There are several measures of that accelerating research progress and its importance, including:

- A global databank of protein structures, which in 1995 had some 3000 entries, in 2010 60,000 entries, and at the end of 2020 more than 155,000 entries, of which 88 percent were based on X-ray studies at major synchrotron research facilities.
- Another measure is the response to viral pandemics, since the outer structures of viruses that determine their infectivity are composed of proteins: the SARS outbreak in 2004 led to 20 entries in the protein database over three years; the Covid outbreak has led to more than 1000 entries in 2020 alone.
- The scientific importance of understanding protein structures and related molecular machines—and hence their biological functions—can be gauged by the award of seven Nobel Prizes for such work over this 25-year period, all of which were enabled by synchrotron X-ray studies.
- The commercial and public health importance can be measured by the flood of new medicines and therapies entering the marketplace that are either protein-based or depend for their effectiveness on attaching to proteins—including the novel Covid antibody vaccines developed in 2020.

What catalyzed and enabled this explosion of research was a new generation of synchrotron X-ray sources built and operated by the Basic Energy Sciences Office of the U.S. Department of Energy as well as similar facilities in Europe and Asia. Synchrotrons—circular magnetic storage rings that accelerate electrons to near the speed of light, then deflect them as X-rays into experimental stations or beamlines—had been used for both physical and biological research since the mid-1970s. The new, third-generation synchrotrons that started to come on-line in 1997 had more intense X-ray beams and were equipped with more experimental stations to support research. DOE ultimately created 4 such shared-use synchrotrons—two in California, one near Chicago, and one at Brookhaven in New York State—as well as an X-ray laser facility (also in California). Moreover, an interagency working group convened by the White House Office of Science led to a ground-breaking memorandum of understanding between DOE and the National Institutes of Health (NIH). The result was that NIH pays for beamlines dedicated to biological research. DOE's Office of Science also created partnerships with groups of pharmaceutical companies, which support beamlines used for proprietary X-ray studies of potential drugs.

That planning and leadership enabled the explosion of research into protein and larger macro-molecular structures and the role they play within living things. In effect, the synchrotron X-ray facilities became a kind of molecular observatory, where university scientists or pharma researchers could ship protein crystals of interest to the lab by Federal Express and get back structure data within a few days. Pharma companies now use these facilities to screen over 20,000 potential drug candidates a year. When the Covid pandemic hit, that capability for remote access turned out to be critical, and has resulted not only in detailed structures of the virus spike proteins but also in half a dozen new Covid drug therapies now in clinical trials.

The Nobel awards illustrate the range and importance of these X-ray investigations of protein and related structures. A 2012 Nobel

This aerial view illustrates the enormous scale of the recently upgraded Brookhaven National Laboratory's X-ray synchrotron. Electrons travelling near the speed of light in the circular magnetic storage ring are converted into X-rays for research use at dozens of individual experimental stations adjacent to the ring.
(SOURCE: BROOKHAVEN NATIONAL LABORATORY)

award, shared by Brian Kobilka, was for research into the structure of the molecular machine known as the G-coupled receptor, to which many drugs attach and which translates such chemical messages into actions within the cell. Crystals of the receptor were hard to make. So the DOE beamline staff at the Argonne National Laboratory synchrotron worked with Kolbilka for many months to develop micro X-ray beams and new ways to focus them on the crystal sample, playing a critical role in the structure determination.

More recently, a 2018 Nobel Prize was awarded Frances Arnold for her work on the directed evolution of enzymes. In effect, Arnold pioneered a bioengineering method that nudges biological organisms to evolve the best enzymes for a given task and condition. She has started three companies to take successful enzymes into the real world. These efforts, based in significant part on X-ray studies (mostly at the SLAC National Accelerator Laboratory synchrotron), include a method of making renewable fuels for planes, trucks, and cars as well as bio-based industrial chemicals; a way to replace agricultural pesticides by making insect pheromones that confuse male bugs and disrupt their mating; and a process that teaches microbes to fuse carbon and silicon, which could remake the massive organosilicon industry that produces sealants, adhesives, and coatings. The potential, Arnold says, is to genetically encode almost any kind of chemistry and let nature carry it out.

Last year a 2020 Nobel Prize was awarded Emmanuelle Charpentier and Jennifer Doudna for the development of extremely precise and programmable genetic editing tools, based on a protein named CRISPR-Cas9. Those ground-breaking tools allow errors in DNA to be corrected and thus potentially create a way to cure—not just treat—inherited diseases such as sickle-cell anemia or cystic fibrosis. In that work, Doudna made extensive use of the synchrotron X-ray source at the DOE Lawrence Berkeley National Laboratory to understand how RNA molecules can guide the flow of genetic information in cells.

Over the past 25 years, however, other countries have also built high-intensity synchrotron X-ray sources. There are now more than 50 such facilities in operation or under construction worldwide. Moreover, the demand for access to such indispensable research tools has grown even faster—current DOE synchrotron facilities cannot accommodate many of the requests for beam time. For the U.S. to maintain its competitive position, and to make the most of the new scientific, medical, and industrial opportunities, may require upgraded beamlines, more beamline staff to assist users, and perhaps additional facilities.

Neutron Sources

The United States is also yielding its world leadership in neutron sources, even though neutron scattering and other techniques available only at these sources are essential to high-impact science and engineering research and crucial medical and manufacturing processes.

While the Spallation Neutron Source positions the U.S. as one of the leaders in pulsed, spallation sources, a recent report[5] by the BESAC Subcommittee to Assess the Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility laid out the pressing need to shore up this nation's limited neutron source capabilities. Substantial investment is needed, both in new facilities and next-generation instrumentation, to support the U.S. research enterprise. The report recommends that these efforts should include upgrading the existing high-performance research reactor and development of new reactors and designs to replace aging infrastructure and thereby retain their ability to deliver research and isotope production critical to the nation.

5. *The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility*, DOE Office of Science, 2020

Researcher Eric Gibbs from St. Jude Children's Research Hospital uses neutrons at Oak Ridge National Laboratory's High Flux reactor to study proteins that suppress cancer tumors.
(CREDIT: GENEVIEVE MARTIN/ORNL)

3. STRATEGIES FOR SUCCESS, RECRUITMENT, AND RETENTION

In the context of this international benchmarking study, success would mean, at a minimum, improving the status of U.S. basic energy science in terms of the metrics and consultations that have been employed in this study. A full embodiment of success is to achieve competitive status as described in the 2000 NASEM report, *Experiments in International Benchmarking of U.S. Research Fields.*[6] The standard for desirable levels of success articulated in that report is two-tiered: (a) First-tier. The United States should be *among* the world leaders in all major areas of science, meaning not substantially exceeded elsewhere; and (b) Higher-tier. The United States should maintain clear leadership in some key areas of science. Meeting the first-tier standard of among the world leaders enables the U.S. to extend and capitalize on important scientific advances in any field no matter where in the world they are made. Meeting the higher-tier standard of clear leadership is necessary for areas in which there are explicit national objectives and for areas in which there are multiple vital areas of application of research results for societal benefit. This report finds that, in the U.S., quantum materials and quantum information science, sustainability research, and the quality of advanced research facilities should meet the higher-tier standard (see Box 3.1. Competitiveness in Quantum Materials).

The results of the quantitative metrics on publication citations and conferences support the judgment that neither of these standards of success is currently met in a satisfying way. So does the more qualitative information gained by the nearly sixty individual consultations in this study. The aim of this section is to suggest actions that could improve the status of U.S. basic energy science. It is not possible to say how far or how fast improvement could occur, but achieving the desired two-tier competitive status is likely to require sustained implementation over a timescale of a decade and beyond.

It is important to recognize that the DOE Office of Basic Energy Sciences has an extensive, well-developed and effective system of Basic Research Needs (BRN) workshops to identify areas for research investment that regularly lead to Funding Opportunity Announcements. That office also receives guidance in the form of priorities for Energy Frontier Research Centers and other centers such as Energy Innovation Hubs and Quantum Information Science Research Centers. This is a proven, successful system for identifying compelling areas of science for investment. The Office of Basic Energy Sciences also maintains an extensive network of advanced research facilities and national laboratory core programs that provide key enabling capabilities and provide continuity for focused efforts. This chapter proposes possible strategies for success that are not explicitly addressed by BRNs.

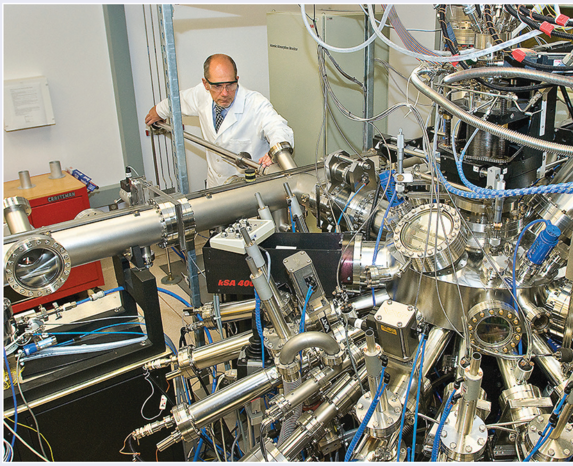
Among the recommendations to achieve a higher level of success that emerged from this study, three main points stand out:

- Increased levels of support for early-career and mid-career scientists, more comparable to those available in Europe, would be desirable to attract and retain talent.
- Increased responsibilities and opportunities for staff scientists at advanced research facilities and national laboratories would permit richer scientific careers and could help retain talent and encourage innovation at those facilities.

6. NASEM 200 report: www.nap.edu/catalog/9784/experiments-in-international-benchmarking-of-us-research-fields

BOX 3.1. COMPETITIVENESS IN QUANTUM MATERIALS

Why physicists had to become materials scientists to explore quantum science



Ivan Bozovic with the atomic-layer-by-layer synthesis system he developed and uses at Brookhaven National Lab to engineer superconducting materials one atomic layer at a time.
(CREDIT: BROOKHAVEN NATIONAL LABORATORY)

At the scale of individual atoms or sub-atomic particles, the behavior of matter is governed by the complex laws of quantum mechanics. That interests physicists, but quantum phenomena have been effectively invisible to most human concerns. That is starting to change, however, because researchers are finding a growing number of quantum effects in macroscopic materials—effects which could have important technological applications. High-temperature superconducting materials that can transmit electrical currents without any losses, for example, could potentially help stabilize electrical grids or enable smaller, lighter generators atop wind turbines. Some two-dimensional materials—composed of layers that are each one atom or molecule in thickness—have unique magnetic or electronic properties and may replace silicon for many IT applications.

Such macroscopic quantum phenomena are still not fully understood. To study these phenomena, however, requires large and extremely pure crystals of relevant materials. And growing such crystals is almost an art form; you can't order them from a supply catalog. That's why physics departments in a number of U.S. universities and in some Department of Energy national laboratories train and maintain cadres of crystal-growing experts as an essential part of their fundamental research efforts. But it wasn't always so.

The invention of the transistor at Bell Laboratories launched the semiconductor industry and established the importance of high-quality single crystals of silicon and other materials. Bell Labs employed experimental physicists to analyze the properties of novel crystals, but they also nurtured people who could grow those crystals. Some were chemists, others started as technicians; but they were all treated as professionals, says one former employee, because they were critical to the innovation process that made Bell Labs a legend. A side benefit of that effort to create and then analyze new materials was that the U.S. led the world in the emerging area of quantum materials, because a generation of U.S. physicists interested in studying quantum phenomena could depend on Bell Labs for high quality samples.

Just how dependent became evident when research on high temperature superconductors accelerated during the 1990s. By then, Bell Labs' crystal-growing capacity had effectively shut down, and physicists trying to investigate and understand high temperature superconductivity had to turn to Japan for high quality crystal specimens. Recognizing that a domestic crystal-growing capability was critical, several leading university physicists began in the late 1980's to jump-start that capability by changing the culture in the physics departments where they worked. At MIT, for example, Marc Kastner and Robert Birgeneau persuaded the university to fund a new crystal-growing laboratory and began to train their students in the art of crystal-growing. Later Birgeneau replicated that effort at the University of California at Berkeley. Other U.S. universities began similar efforts. But real change took decades.

One young scientist's career illustrates what was required to regain a competitive U.S. capability in quantum science. Joe Checkelsky graduated from Princeton in 2004 with a doctorate in low-temperature physics. He wanted to study the electrical properties of materials, but found that the best opportunities to do so were outside the U.S. So he went to Japan for four years, first as a postdoc and then as a faculty member at the University of Tokyo. He found a culture very different from most U.S physics departments. In Japan, there is no distinction between crystal growers and physicists—indeed, graduate students and post docs were routinely trained in crystal growth, and success in crystal growing was a well-established route to gaining tenure at a Japanese university. Joe also found that advanced techniques of crystal growth and materials synthesis had opened up a whole new field of science. In effect, he realized, "where new physics discoveries come from is new materials."

When Joe returned to the U.S., MIT hired him to build a new laboratory that would both grow crystals and study their properties. What emerged is a unique integrated facility—one large space, half devoted to materials synthesis, the other half to advanced measurement—that is staffed by senior people but also trains students in both skills. Similar things happened at other universities too. The Moore Foundation understood the importance of their efforts and became a significant funder, helping universities hire crystal growth talent and obtain the specialized equipment needed. The Department of Energy's Basic Energy Sciences office also funded the effort, as well as creating crystal growth facilities at several national laboratories.

Over the last decade, the impact has been to re-establish at least some degree of U.S. competitiveness in the ability to create the materials required for quantum research. Senior physicists point out, however, that the U.S. does not dominate the field: Japan, Germany, and China all have very competitive capabilities. That loss of leadership is important, given the science and potential new technologies coming from research into quantum materials. For example, the most successful efforts to build practical quantum computers—exponentially faster for certain problems than conventional computers—depend on quantum materials. The advances made possible with such computers are expected to transform information processing for both civilian and defense applications. For both the IT industry and for national security, the stakes in quantum materials are very high.

- Encouraging and permitting more sophisticated integration of research across the spectrum from basic to applied to industrial would help accelerate both research and its translation into societal benefits.

Methodology

This study adopted a consultation methodology to learn as much as possible about the strategies and practices—domestically and globally—that are used in organizations among or similar to those supported by the DOE Office of Basic Energy Sciences. This consultation methodology for benchmarking was broadly endorsed by the 2000 report.[7] Consultations were undertaken with fifty-nine individuals representing a broad spectrum of research responsibility including: national laboratory leadership; university leadership; National Science Foundation and private foundation leadership; international leadership in research, facilities, and research management; early career scientists; representatives of user committees of domestic and international user facilities; and domestic and international industry leadership.

A tailored set of questions and discussion points was provided for each consultation, aimed at uncovering strategies, practices, attitudes, opinions and incentives in each type of organization. A first round of consultations produced a consensus set of hypotheses concerning the status of U.S. international competitiveness. A second round of consultations endeavored to test these hypotheses before arriving at the conclusions and recommendations proposed in this report.

Strategy: *Recruitment and retention*

Attracting and retaining human talent is unequivocally crucial to any success strategy. During the second half of the twentieth century, the United States was a magnet for the brightest and best scientific talent from around the world. Thousands of PhD students came to the U.S. from Asia, Europe and Latin America; while many still come from east and south Asia, numbers are down from the rest of the world. U.S. experience was the default option for Europeans and other nationalities for doing post-doctoral training before seeking a permanent position. Many of those who came to the U.S. during this period chose to settle down here, and they became an important and substantial component of the nation's scientific human capital. This helped enable the U.S. to enjoy a period of unquestioned dominance in the realm of scientific discovery and progress (see Box 3.2. The Worldwide Competition for Talent).

Since the beginning of the twenty-first century, however, this situation has gradually changed. There is plenty of evidence to suggest that the recruitment and retention of top scientific talent from around the world has become more difficult for the U.S., especially over the last decade. Broad consultations carried out during this study lead unambiguously to the conclusion that the U.S. is now losing the global competition for talent. Weakness in talent recruitment and retention appears from this study to be one root cause of failure to achieve the desired competitive status for the U.S.

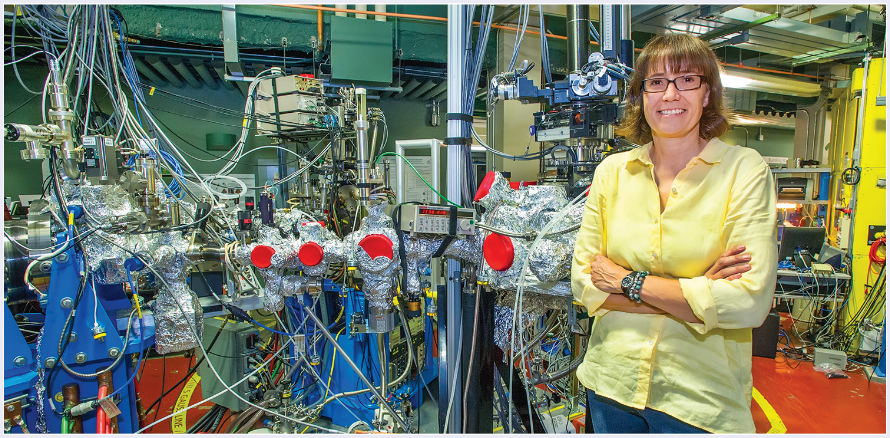
The growth of scientific competition from Asia is strikingly underlined by the *U.S. News and World Report* global university rankings for 2021.[8] Five Asian universities are in the world's top dozen for Chemistry, 10 of 12 for Chemical Engineering, 7 of 12 for Materials Science, 8 of 12 for Engineering, 3 of 12 for Physics and 4 of 12 in Computer Science. Singapore's NUS and NTU feature prominently, as do China's Tsinghua and USTC, among others. NTU Singapore is ranked at the top of world universities in three areas: materials science; energy and fuels; and nanoscience and nanotechnology. Given that this is a U.S.-based ranking that is heavily fo-

7. Committee on Science Engineering and Public Policy, *Experiments in International Benchmarking of U.S. Research Fields*

8. www.usnews.com/education/best-global-universities/rankings

BOX 3.2. THE WORLDWIDE COMPETITION FOR TALENT

Why the U.S. Was a Magnet, but Is Not Anymore



Elke Arenholz with one of the specialized beamline instruments she developed for the Advanced Light Source synchrotron for measuring the magnetic properties of materials (CREDIT: ELKE ARENHOLZ)

In the second half of the 20th century, the U.S. benefited from a steady stream of talented young scientists coming here as graduate students or postdocs. Many stayed, becoming U.S. citizens. One of these was Elke Arenholz, born in Germany where she studied physics. She was attracted to what could be learned about magnetic materials with the X-rays generated by electrons accelerated in synchrotrons, which she thought were "cool machines." She was an outstanding student: her doctoral thesis in 1996 at the Free University of Berlin was recognized as the best that year in all of Germany for research with synchrotron radiation.

The following year, Elke came to the U.S. on a postdoctoral fellowship at the University of California at Berkeley, sponsored by the Miller Institute—attracted both by the chance to visit the U.S. and also because the fellowship generously allowed her to work on a very large range of science questions. At the fellowship's conclusion, she had several options and accepted an offer to work on the newly-installed magnetism beamline of the Advanced Light Source (ALS) synchrotron at the U.S. Department of Energy's Lawrence Berkeley National Laboratory. She chose this opportunity, in part, she says, because she was attracted to the idea of building new and unique research tools and to work with diverse groups of experienced scientists and engineers.

That began an 18-year career at ALS, building new instruments to explore the magnetic properties of materials with soft X-rays, working as part of the scientific support group for visiting scientists at the ALS facility, and conducting her own research. That support effort often turned into close collaborations. She also pioneered a number of new research tools—such as a novel magnet system that significantly enhanced the capability of the ALS to measure magnetic properties of materials. The instruments proved important in the development and characterizing of materials used in computer hard drives. Later she developed new ways to measure the dynamics of magnetic phenomena, following magnetization changes element by element on a nanosecond timescale. She also worked on the use of magnetic nanoparticles to deliver medical therapies inside human bodies, on novel phenomena in quantum materials, and much more.

Dr. Arenholz became one of the world's leading scientists in magnetism, with over 370 publications, many invited presentations at international conferences, and recognition in the form of prestigious awards and memberships. She also became adjunct faculty in the U.C. Berkeley Department of Materials Science and Engineering, while also advancing to deputy head of the ALS support group and later deputy group leader for ALS's Photon Science Operation. In 2019 she moved to Cornell University to become Associate Director of the Cornell High Energy Synchrotron Source (CHESS).

That career is all the more impressive, given that women scientists were (and still are) relatively rare in most areas of physics. Throughout her career, she was often the only woman in the room—which, she says, meant more pressure to be perfect, but also increased her visibility as a scientist. "No one told me you can't do this because you're a woman," she says, and her excitement for the research itself was both sustaining and often helped gain acceptance. She has consistently mentored other women scientists, telling them "just be super-prepared." Her self-confidence and enthusiasm were always evident, says Zahid Hussain, who was head of the ALS scientific support group and hired and supervised Elke at that facility.

It's clear that the U.S. has benefited greatly from her decision to come to the U.S. and to stay here (Germany tried hard to lure her back about midway in her stay at the ALS)—just as it does from the many other talented young scientists who have come to the U.S. in the past. Things have changed, however. As Elke points out, "other parts of the world have learned from the U.S. and provide resources like the fellowship that brought me to the U.S." Both in Europe and in Japan and other parts of Asia, countries have also built world-class research facilities and provide impressive user support for visiting researchers. Moreover, recent uncertainty about U.S. visas for foreign students or visiting scientists has exacerbated the problem.

Indeed, a recent analysis by *U.S. News and World Report*[a] shows that Asian universities, especially in Singapore and in China, now rank highly in many disciplines: among the top 12 in the world, Asia accounted for 5 in chemistry, 8 in chemical engineering, 3 in physics, and 4 in computer science. NTU Singapore is ranked as the leading university in the world in materials science, energy and fuels, and nanoscience.

A more detailed report by the American Academy of Arts and Sciences[b] points to a number of factors attracting a growing number of both junior and senior scientists of foreign origin to leave the U.S. for European or Asian universities. These include increasingly competitive salaries and a sense that the U.S. has become less welcoming to foreigners. Likewise, the lack of consistent support for research careers in the U.S. does not compare well with the generous lifetime support for talented senior scientists offered by leading German research institutions. As a result, there is a worldwide competition for scientific talent, and for the innovations that scientific discoveries can drive—and the U.S. is no longer the winner by default.

a. https://www.usnews.com/education/best-global-universities/rankings

b. *The Perils of Complacency, America at a Tipping Point in Science and Engineering* (American Academy of Arts and Sciences, 2020) cused on research, these rankings strongly highlight the global competition and headwinds for the future of American leadership in science and engineering.

Many factors are contributing to these trends. There has been a marked growth in global demand for top talent, as both established and emerging nations are able to offer attractive career opportunities for their own nationals and, in many cases, foreign scientists. China is the most obvious example because its growing economy has funded a rapid expansion of its scientific infrastructure. Chinese-born scientists in the U.S. can now choose to return to their homeland without sacrificing their standard of living as was the case one or two decades ago. That includes younger scientists who are weighing the relative merits of settling in the U.S. versus returning to their country of origin, as well as scientists who have been in the U.S. for many decades. This trend applies not only to Chinese scientists, however, but also to varying extents to Europeans, Japanese, South Koreans, Russians, and Singaporeans, among others.

Some foreign scientists have been unable to come to the U.S. because of difficulties around obtaining visas and Green Cards over the last few years. This affects not only universities and national laboratories, but also industry. These challenges have been particularly difficult during the pandemic of 2020, though it may change with widespread availability of vaccines.

Other foreign scientists choose not to come to the U.S., or choose to leave, because the country may seem more unwelcoming to people not born in the U.S. than in the past. As a consequence, for example, more Chinese scientists now go to Europe than in the past to acquire international experience.

The attractions of moving to, or staying in, Europe have increased in recent years, in part due to excellent funding opportunities through five-year European Research Council (ERC) grants for single investigators (both junior and senior), as well as generous long-term funding that is offered by the German Max Planck Institutes and the Swiss Federal Schools, among others. The same is true in relation to several Asian countries. These generous, long-term funding mechanisms have been emphasized in several of the consultations carried out by members of the International Benchmarking Subcommittee.

Of course, many scientists choose to move back to their homelands for purely personal reasons, such as to be closer to family, friends and familiar circumstances, though this is not a factor that is new during recent years.

In response to the global competition to attract or retain top talent, several countries have launched schemes aimed at bringing back their diaspora, while other nations are competing for mobile international talent. Many do both. There has been much discussion in the U.S. about China's 1000 Talents Plan, which has programs for both young and senior Chinese scientists from the U.S. and elsewhere, as well as one for foreign talent. Many examples were cited and tabulated in consultations. The consultations also suggest that the number of high visibility losses to China is still quite small in the physical sciences and engineering, possibly because it can be difficult to adapt to the Chinese culture after spending many years in the U.S. However, the situation may change rapidly, so the U.S. should not be complacent. At the same time, large numbers of younger Chinese scientists leave the U.S. each year because there are more opportunities for them in China and, for a variety of reasons, it can be difficult for them to secure permanent positions in the U.S.

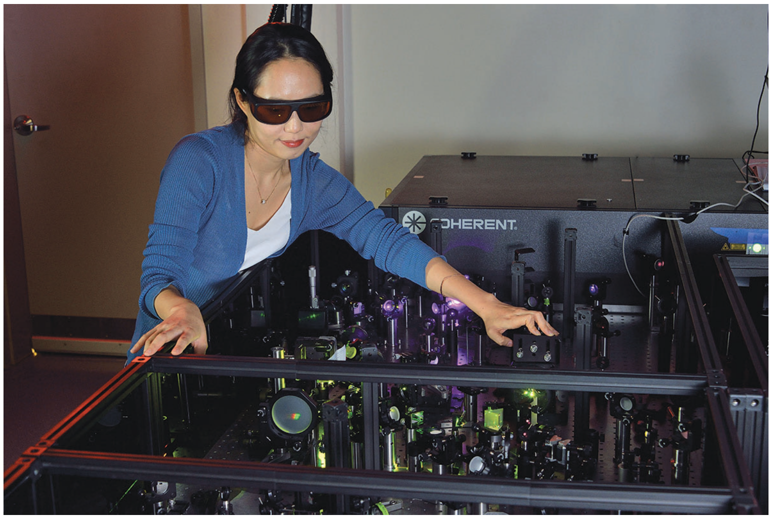
It is important to recognize that China's 1000 Talents program is by no means unusual in the global landscape, and it would be a mistake to regard China as being the only threat to American leadership in basic energy sciences. For example, the Returning Singaporean Scientists Scheme *"seeks to attract outstanding overseas-based Singaporean research leaders back to Singapore to take up leadership* *positions in Singapore's autonomous universities and publicly funded research institutes.*" As the balance of scientific power, propelled by strong and sustained investments in R&D as well as a highly trained pool of talent, shifts gradually towards Asia, there is growing evidence that countries such as Singapore are able to compete with the U.S. and Europe for the top international talent. While Singapore is a very small city-state with a small population and talent pool, the rise of other Asian economies and the resultant increase in their scientific output, including those of ASEAN, India and China, will inevitably pose a serious challenge for the U.S. in talent attraction and technological leadership unless some of the current trends can be reversed quickly. These sentiments are also reflected in the detailed report from the American Academy of Arts and Sciences.[9]

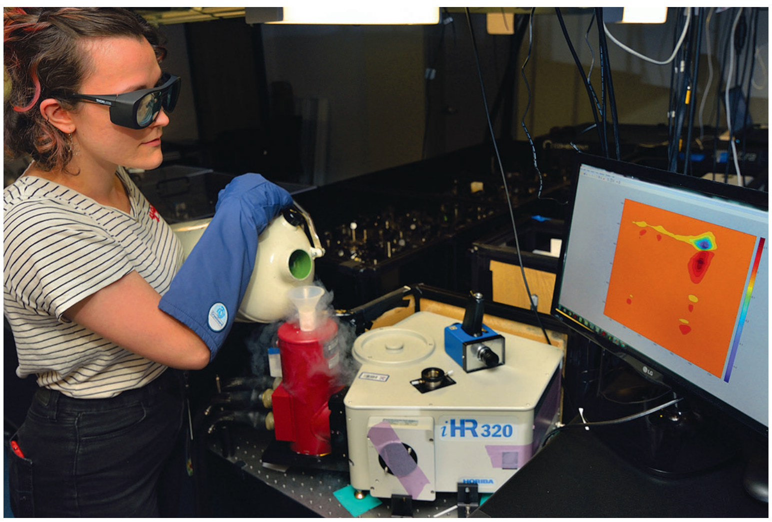
Other nations that are competing for mobile international talent include Australia, Canada, the UK, South Korea and Germany. The Australian Laureate Fellowships program and the Canadian Research Chairs program have been running for several years. These schemes typically offer a number of attractions, including salary supplements and substantial research support. In the case of the Canada Research Chairs, Canada invests up to $295 million (Canadian) per year to "attract and retain some of the world's most accomplished and promising minds." The more senior Tier 1 Chairs can be held for a maximum of *two consecutive seven-year periods*, so they can provide stable, long-term funding. There is also a more exclusive program of Canada Excellence Research Chairs, which is restricted to senior people coming to Canada from elsewhere. These offer $10 million (Canadian) over seven years. Beyond that, there is a new Canada 150 Research Chairs program that is part of the country's 150th anniversary. These seven-year awards can be worth up to $1 million per

Sheng Dai is a prolific senior researcher at Oak Ridge National Laboratory who studies chemical separations, nanomaterial synthesis, and catalytic interfaces for energy applications; he also heads a DOE Energy Frontier Research Center on interface reactions.
(CREDIT: ORNL)

year. The UK, too, has a range of instruments that aim to attract its diaspora as well as foreign talent, and will be doing even more in this area in the aftermath of Brexit. For example, the UK's national academy, the Royal Society, offers a number of Royal Society Research Professorships each year that provide support over a period of up to 10 years. South Korea created the Institute of Basic Science (IBS) in 2011 and now operates 31 Research Centers that span many key areas of modern science and technology. Korea has used the resources of the IBS to attract global leading senior scientists as Directors of these Centers. It also offers fellowships to attract outstanding young scientists. Germany, too, has a national scheme for attracting talent. The Alexander von Humboldt Professorships offer an award of €5 million over 5 years to draw top international researchers to German universities. The federal schools in Switzerland—ETH Zurich and EPFL Lausanne—also offer very attractive, long-term funding for their faculty members and both institutions have successfully attracted senior faculty from U.S. universities. (In some cases, these moves involve people who originally moved to the U.S. from Europe.) The U.S. has not entirely lost its allure, though the number of senior people leav-

9. *The Perils of Complacency, America at a Tipping Point in Science and Engineering* (American Academy of Arts and Sciences, 2020), www.amacad.org/publication/perils-of-complacency





Advancing the understanding of solar energy conversion requires the use of advanced tools. For example, the ultrafast laser spectroscopy equipment shown here is a laboratory-scale tool in the UPenn lab of Prof. Jessica Anna (a DOE Early Career Recipient) that allows for the investigation of energy and electron transfer, two fundamental processes that govern solar energy conversion. Graduate students Dabin Kim (top) is aligning the visible laser spectrometer and Phoebe Askelson (bottom) is cooling a detector with liquid nitrogen to perform spectroscopy measurements. (CREDIT: FELICE MACERA, UPENN)

ing is certainly greater than those who are coming here, as amply documented by the consultations for this report.

The above summary of international opportunities is not exhaustive, but clearly shows that there is enormous, multi-faceted global competition for top scientific talent. This has been confirmed and reinforced by consultations with dozens of individuals in the U.S. and abroad, and at all career stages ranging from early career scientists to leadership of national laboratories and universities. The United States has not generally offered such schemes, depending instead on a constant influx of foreign scientists. However, this study confirms that influx does not automatically lead to retention and, in fact, that retention is diminishing. Accordingly, this report suggests that the U.S. and the Department of Energy, in particular, cannot afford to ignore this global competition—and that it may be time to take action in order to preserve and, in some areas, restore the nation's scientific leadership in basic energy sciences.

There are significant issues at both the junior and senior level. At the junior level, the DOE's Early Career Research Program offers about 50 awards to university investigators each year with an average value of $750K over five years and another 30 or so to national laboratory investigators at $2.5 million over five years (a substantial fraction of which goes to support the investigator's salaries and to indirect costs at the laboratories). This is less compelling compared to the European Research Council (ERC) Starting Grants of up to €1.5 million (~$1.8 million) for a period of 5 years. Moreover, the ERC awards approximately 450 such grants each year (with approaching 50% of them in physical sciences and engineering). An additional €1 million can be made available to cover start-up costs and/or the purchase of major equipment and/or access to large facilities and/or other major experimental and field work costs. Another attractive feature is that the ERC's grants operate on a 'bottom-up' basis without predetermined priorities, in contrast to the DOE's Early Career Research Program. Finally, we note that there is no follow-on opportunity with DOE's Early Career Research Program, whereas the ERC has an annual offering of more than 300 mid-career Consolidator grants of up to €2 million value over 5 years.

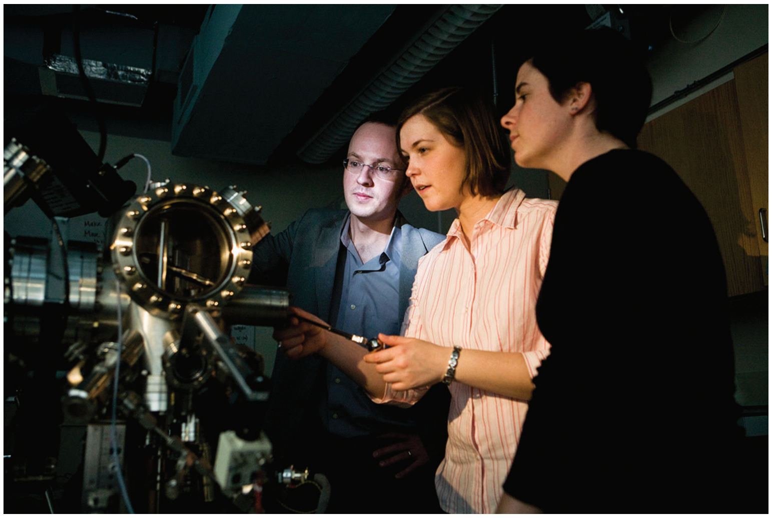
The absence of follow-on opportunities with DOE's Early Career Research Program is part of a more general issue with the U.S. funding model for mid-career and senior scientists in the physical sciences and engineering. Unlike the life sciences, where, for example, the Howard Hughes Medical Institute supports nearly 300 HHMI Investigators in the U.S. on a seven-year renewable basis with a value of around $1 million per year, there are *virtually no opportunities* for physical and engineering scientists to obtain single investigator funding for more than three years at a time. The only way to avoid this is to become part of a larger team. This is particularly striking in the national laboratories, where it is extremely difficult nowadays for a scientist to pursue a top-class career as an individual investigator. By contrast, the ERC gives around 200 Advanced Grants for individual investigators each year, with a value of up to €2.5 million for a period of 5 years, and there are similar schemes in several other countries. A troubling number of top scientists in the broad basic energy sciences area have left U.S. institutions in recent years for such opportunities in Europe. While the number of such people is not very large, they are among the top people in their respective fields. (The loss of senior, well-established people to Europe is more severe than to Asia, and those leaving to Europe are nearly all of European origin).

Historically, the hospitable environment for international scientists in the U.S. produced the most internationally diverse cadre of researchers anywhere in the world. That international diversity has been an advantage both in the numbers of talented people it brought to the U.S. and in different kinds of training and cultural connections they brought with them. This international diversity advantage is now under threat and vulnerable, unless steps can be taken to provide a more hospitable environment for all scientists.

Recommendations. This report finds an urgent need to establish programs that will enable the U.S. to continue attracting and retaining top talent from across the world. That in turn provides an opportunity for the Department of Energy to play an important role, as the leading agency for energy-related physical science and engineering research.

The main elements of the programs offered by our competitors are: (i) sustained research funding for individual investigators at all career levels that enables them to focus on challenging problems for a significant period of time (for a minimum of 5 years and in many cases up to 10); (ii) less emphasis on top-down area guidance on areas of research for Early Career Awards; (iii) where possible, reduction or elimination of teaching duties to free up more time for research; (iv) enhanced salaries to reflect the prestige of the positions. (Elements (iii) and (iv) are more in the hands of the institutions than the funding agency, and it is also pertinent that some of the suggestions below must be tailored differently for national laboratory and university researchers.)

There are several possibilities to consider. One suggestion would be to substantially increase the mean value of DOE's Early Career Awards to $1.5 million over 5 years to university investigators and $5.0 million over five years for national laboratory investigators. If compromises must be made, the suggestion is to favor the enhancement for national laboratory scientists whose options for building a career as principal investigators are more limited than those for university scientists. DOE should consider allowing the program directions to be decided from the bottom up, rather than constrained in area by program managers. At both universities and national laboratories, consideration should be given to investment in the Early Career Awardees who have been demonstrably the most success during the five-year term of their award. A follow-on opportunity for Early Career Award holders so that at least half of them can secure funding at the same rate for a further five years would be desirable. Several consultations also suggested that placing serious responsibility into the hands of early career scientists would



Imaging at the level of atoms and molecules is critical to the area of nanoscience. The development of new laboratory-scale tools, including the scanning tunneling microscope in the Tufts University laboratory of Prof. Charles Sykes—pictured here with former graduate students April Jewell (NASA Jet Propulsion Lab) and Erin Isk (Associate Professor, University of Tulsa)—have played an important role in advancing basic energy research and in workforce development. Sykes' research provides key insights into the function of new nanoscale catalysts. (CREDIT: TUFTS UNIVERSITY)

act as an important retention measure. Support for career development of early career scientists at national laboratories is especially needed to attract talent to this important element of the nation's scientific workforce.

To address directly the international competition for recruiting and retaining talent at the senior level, creation of DOE Senior Investigator Awards at a level of up to $5 million over five years would create exciting opportunities for top single investigators in the basic energy sciences, whether at national laboratories or universities (though the award amounts should be adjusted to yield similar direct funds available to the investigators, despite different indirect cost structures at different institutions). A certain fraction of these (maybe 20%) might be set aside specifically to assist recruitment of non-U.S.-based international talent to U.S. universities and national laboratories. The aim is to reverse the direction of the efflux of talent out of the U.S. We emphasize that these enhanced investments are specifically aimed at talent recruitment and retention; however, it is clear from this study and others (*American Academy report*[10]) that there are strong correlations between the levels of financial investments in research and the quality, visibility and impact of the research.

Strategy: *Management and support of facilities*

After human scientific talent, the next most important investment in the U.S. basic energy science research enterprise is that for advanced research facilities. The research results enabled by these facilities contribute greatly to the competitive status of U.S. science. Facilities attract talent from around the world as users and collaborators. Just as for human scientific talent, there is international competition in facilities in terms of their capability, their capacity and their scientific impact. This study has shown, through both literature citation data and through numerous consultations within the U.S. and internationally, that the capability of BES facilities is generally at a high level, but their scientific impact, and their capacity, is losing or has lost leadership internationally.

Facilities here refers to the advanced research facilities supported by the Office of Basic Energy Sciences, including synchrotron and free electron laser X-ray sources for X-ray scattering, reactor and spallation neutron sources for neutron scattering, electron microscopy facilities, and nanoscale science centers. Access to computational facilities and the software and algorithm tools to use them effectively is also increasingly important. Though we have not studied the situation with computational facilities as extensively as the physical facilities, there is evidence from consultations and from notable loss of senior scientists that Europe is in a stronger position in scientific computation.

10. *The Perils of Complacency, America at a Tipping Point in Science and Engineering* (American Academy of Arts and Sciences, 2020), www.amacad.org/publication/perils-of-complacency

Domestic and international consultations in this study have led to the idea that facilities with highest impact on science have several common characteristics. They enable facility staff to think creatively, independently and big, and to develop new research directions and tools. In so doing, they develop an environment in which outstanding scientists both interact with users, develop new instrumentation, and can have careers themselves of growing impact and accomplishment. They have intellectual engagement with, as well as providing expert help to, users. They perform training and knowledge dissemination functions that produce broad engagement and awareness of the capabilities within the community.

Generally, the access of a user to a facility, after acceptance of a proposal for time, is through the intermediary of a beamline scientist or analogous facility scientist for electron microscopy or nanoscience. These are the facility-based scientists to whom the preceding paragraph refers. According to the results of numerous consultations in this study, the characteristics of high impact facilities outlined in the preceding paragraphs are not usually in place at U.S. facilities, and are more the rule at international facilities, especially European. There also seem to be competitive deficits in U.S. facility capacity, most notably in neutron scattering *vis-à-vis* Europe. This capacity shortage in neutrons is exacerbated by the temporary shutdown of the NIST Center for Neutron Research (NCNR) reactor and the need to upgrade or replace the HFIR facility at ORNL.[11] Similarly, the U.S. has no electron microscopy facility as well-equipped as the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons in the Forschungszentrum Jülich (Germany) belonging to the Helmholtz Association of German Research Centres.

There seems to be a general sense from the consultations in this study that, compared to international competition, U.S. facilities are able to attract excellent people, but the investments in the tools and operations of the facilities are less. The 2013 Report of the BESAC Subcommittee on Future X-ray Light Sources[12] positioned the Office of Basic Energy Sciences to invest capital in LCLS (and further free-electron laser X-ray facilities such as LCLS-II and LCLS-II-HE), and in upgrades to the APS and ALS synchrotrons. Continued long-range planning and maintaining strong facilities infrastructure is essential and the Office of Basic Energy Sciences has generally performed well in this respect (see Box 3.3. Why Long-Range Planning is Critical to U.S. Competitiveness). However, new investments and longer-range planning in human resources, instrumentation, operational innovations and science programs at facilities are less evident and are needed.

Recommendations. Though significant investments in light sources and neutron facilities have been made or are contemplated, this report suggests that additional capital investment in electron microscopy, nanocenters, and computational facilities should be considered. Another idea emerging from this study, which might serve to keep U.S. facilities at the leading edge, would be to pursue opportunities for constructive engagement between the DOE Office of Basic Energy Sciences and accelerator science in areas from electron microscopy to light sources. And while there have been several collaborative initiatives between that office and Advanced Scientific Computing Research within DOE, this report suggests that the need is more urgent than ever for constructive engagement between the basic energy sciences and advanced computing in areas as diverse as artificial intelligence and 'big' data analy-

11. *The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility,* DOE Office of Science, 2020. www.science.osti.gov/-/media/bes/besac/pdf/Reports/Future_Light_Sources_report_BESAC_approved_72513.pdf

12. www.science.osti.gov/-/media/bes/besac/pdf/Reports/Future_Light_Sources_report_BESAC_approved_72513.pdf

BOX 3.3. WHY LONG-RANGE PLANNING IS CRITICAL TO U.S. COMPETITIVENESS

Discovering the chemistry that enables life on Earth

More than three billion years ago, cyanobacteria, the evolutionary predecessor of plants, learned how to use sunlight, water, and carbon dioxide from the air in a series of reactions that create sugar and release oxygen into the atmosphere. As plants evolved and oxygen levels in the atmosphere increased, it enabled the evolution of more complex life forms, eventually including human beings. Yet scientists are only now learning—with the help of a transformative research facility—how the critical, life-enabling chemical reaction occurs: how plants split a water molecule (H_2O) to release oxygen.

Innovative research facilities have been the hallmark of the Department of Energy's Office of Basic Energy Sciences for over 40 years: from the first major synchrotron X-ray sources at several national laboratories in the 1980's, to increasingly powerful supercomputing facilities at Oak Ridge National Laboratory and elsewhere, to the newer nano-science centers. But the creation of the world's first X-ray free electron laser (XFEL) at the SLAC National Accelerator Laboratory—the facility that made possible the water-splitting research and much else—is a remarkable story in itself.

Lasers that emit infra-red or visible light have been familiar tools for a long time, but it was widely believed that X-ray lasers—which would have extremely short wavelengths, about the width of an atom—were not possible. In the early 1990's, however, Claudio Pelligrini published theoretical research suggesting such lasers might indeed be possible, if powered by SLAC's miles-long linear accelerator, and thus might be used to examine and characterize materials during the course of a chemical reaction literally atom by atom. SLAC proposed to DOE's Office of Basic Energy Sciences a modest pilot-scale effort to test the concept. That office, then led by Pat Dehmer, understood how transformative such an instrument would be for scientific research, and after careful study, proposed to build a full-scale instrument and user facility: a huge bet on unproven technology that paid off, and a powerful example of DOE leadership.

The XFEL took 10 years to build and required a novel and very intense electron source as well as precise alignment of superconducting magnet rings over the entire length of the accelerator. But when it was turned on, it worked even better than had been expected: electrons accelerated almost to the speed of light, which in turn generated intense, extremely short pulses of X-rays 100 times a second. Those pulses, in turn, enabled a series of snapshots of an experimental sample—each taken in less than a tenth of a trillionth of a second—that effectively create atomic-scale movies of chemical reactions or viral protein motions. So productive has this pioneering U.S. facility been that it has since been copied in Germany, Switzerland, Japan, and Korea, with one in China nearing completion. Persis Drell, who led SLAC when the XFEL began operations in 2010, says that the leadership and long-term planning by DOE were critical.

SLAC 2-mile linear accelerator tunnel, part of which has been remade into the XFEL X-ray laser (CREDIT: SLAC NATIONAL ACCELERATOR LABORATORY)

The water-splitting reaction involves a plant protein molecule containing a cluster of 4 manganese atoms, which—together with sunlight—catalyze the reaction; indeed, every leaf on every green plant churns out oxygen almost continuously when the sun is shining. The decade-long international research effort using the XFEL to understand the reaction—led by scientists at DOE's Lawrence Berkeley National Laboratory and including researchers from SLAC, Germany, Sweden and other countries—involved many stages. It required learning how to prepare micro-crystal samples of the plant protein contained in tiny liquid droplets; the liquid droplets are essential, because the reaction only takes place—and thus has to be studied—at room temperature, not with frozen crystals. The researchers also developed a method of launching these micro-droplets of liquid onto a conveyor belt by sound waves, so that they arrive in the right place at the right time. And they created a laser with the exact optical characteristics needed to initiate the water-splitting reaction in each droplet.

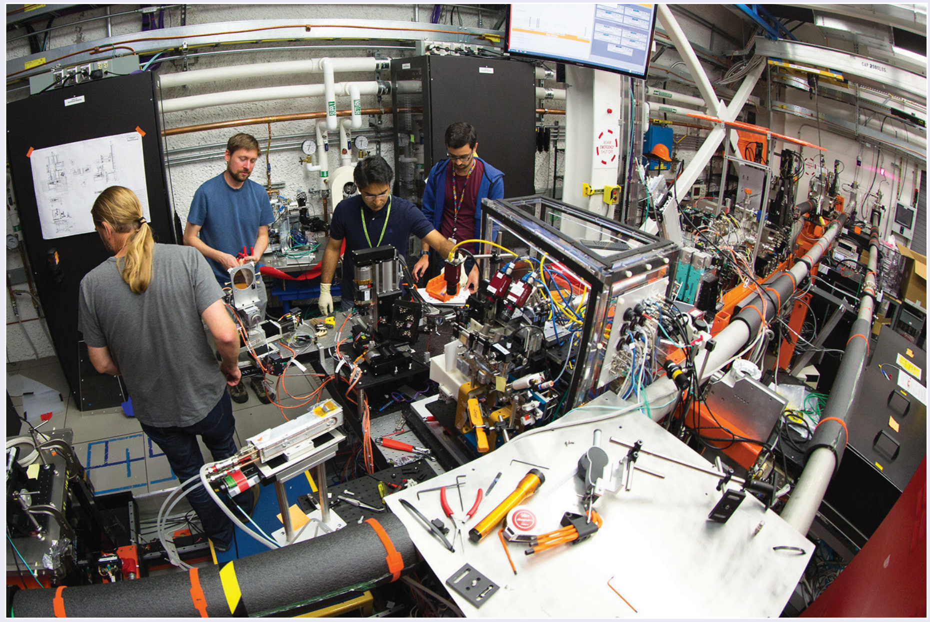
When the experiment is running at the XFEL, it requires precise coordination of X-ray pulses, ejection of the sample droplet, firing the laser pulse, and measurements by two types of detectors. That enables simultaneous measurement of both the position of each atom in the protein (by a technique known as X-ray diffraction) and the chemical state of the manganese atoms (by a technique known as X-ray emission spectroscopy), before the sample is destroyed by the intense X-ray pulse. The final step is the synthesis and analysis of data from hundreds of thousands of samples.

The result has been a series of snapshots that show how the atoms in the manganese cluster rearrange both their positions and their chemical states to split off oxygen atoms from two water molecules and bring them together to form an oxygen molecule. Analysis of the data have led to a now nearly complete atomic-level understanding of the water-splitting reaction—a remarkable piece of basic science. And when the reaction is fully understood, then it might also be possible to make synthetic versions using manganese or similar catalysts, and use them to produce hydrogen or other modern fuels on an industrial scale--directly from sunlight and water.

Equally, however, this research illustrates how important long-range planning and financing for new, cutting-edge research facilities—such as the XFEL—is for continued U.S. leadership in an increasingly competitive world. Besides X-rays, neutrons are the other primary tool for studying the structure of matter. And the

BOX 3.3. *continued*

High Flux Isotope Reactor (HFIR) at DOE's Oak Ridge National Laboratory is the world's most intense source of neutrons outside Russia. But it faces several impending challenges. The reactor is more than 55 years old and will need a new pressure vessel within a couple of decades to avoid failure. To comply with an international treaty, it must switch to a low-enriched uranium fuel. And it badly needs additional capacity—both additional beamlines for researchers and more capacity for production of radioactive isotopes, including those urgently needed for national security applications that are not obtainable from any other source. A recent BESAC report[a] in fact recommends that all three issues be dealt with at the same time, to avoid repeated lengthy shutdowns; or else that an entirely new reactor be built as a replacement. Since either approach will likely take a couple of decades, the report urges that planning begin promptly.



The experimental setup for documenting the chemistry of the water-splitting reaction at the XFEL X-ray laser
(CREDIT: SLAC NATIONAL ACCELERATOR LABORATORY)

a. *The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility,* DOE Office of Science, 2020

sis. (See Box 3.4, How Data-Driven Science is Helping Combat the Covid Crisis).

These are the simple parts, at least in principle. If the characteristics of high impact facilities described above are correct, then several further actions should also be considered. Information developed in this study suggests that the job description and work environment of beamline or other facilities scientists should go beyond service and assistance to users, and should also include adequate time and resources for these scientists to engage in significant, creative science themselves. This will not be simple or straightforward, since there are different types of facilities. Even within one type, synchrotron X-ray facilities, some beamline scientists are employed by the facility and some are employed by collaborative access teams financed by other agencies or entities. Considering this diversity and the desire to generate more high impact science from research in which facilities are an essential component leads to the suggestion that the Office of Basic Energy Sciences undertake or commission a thorough analysis of the job descriptions, scientific productivity, and career paths of facilities scientists. The goal would be to create in all U.S. advanced research facilities those characteristics that create the highest impact on science.

BOX 3.4. HOW DATA-DRIVEN SCIENCE IS HELPING COMBAT THE COVID CRISIS

The growing importance of powerful computers and software algorithms in research

The world has experienced at least 4 major virus outbreaks in the past decade: Covid-19, Zika, Ebola, MERS. Understanding their complex protein structures—especially the protein that enables them to attach to human cells—has been critical to the ability to create vaccines and therapies. This progress has involved both powerful new imaging tools and techniques developed over the past several decades, and the emergence of a fundamentally new kind of science powered by artificial intelligence algorithms.

The imaging tool, called cryo-electron microscopy (cryo-EM), uses electrons to look at molecules quick-frozen in solution, resulting in 3-D images that can now reveal even the positions of individual hydrogen atoms—far beyond what light-based microscopy can do. But initially, before the cryo-methods were available, the tool was applied to air-dried, stained samples of molecules ordered in crystals and the resulting 3-D images were often fuzzy. A key breakthrough came when Joachim Frank of Columbia University began to image thousands of individual molecules, eventually using samples quick-frozen in solution. Each image came from a molecule viewed in a random, unknown orientation. Frank used an image processing system developed to enhance images from planetary flyby missions as a framework to develop his own unique system for combining 2-dimensional snapshots into 3-dimensional structures of individual molecules. He then built computer programs to systematically process raw cryo-EM images into 3-D structures. As computers became more powerful, the image-processing programs also evolved and improved over time.

A revolutionary hardware development came in about 2012 when recording of molecular images on film was replaced by powerful digital detectors—effectively electron-counting cameras--able to record individual electrons reflected from a sample. Developed by scientists from the U.S. Department of Energy's Lawrence Berkeley National Laboratory and from DOE's nano-scale research centers, these new tools were quickly applied to cryo-EM research. That led to publication of the first atomic-level three-dimensional protein structure, and, a few years later, a Nobel Prize in chemistry (awarded to Frank and two others) for the development of cryo-EM.

However, protein molecules are not rigid static structures: they are microscopic biological machines that bend and twist and fold, and whose dynamics are important to their biological functions. In the case of the Covid-19 spike protein, for example, these movements are thought to play a key role in how the virus infects a human cell. As in fly-fishing, where the motions of the hook are decisive, the motions of the spike protein play a similar role.

More broadly, documenting the actions of proteins and other biological machines opens up a new era for molecular biology and has required a set of new tools from data-driven, artificial intelligence approaches to research. Work pioneered by a group of Frank's collaborators--supported by the U.S. Department of Energy's Basic Energy Sciences office over more than a decade—has led to a blossoming of machine learning algorithms for scientific applications. These algorithms can interpret images of proteins frozen in random stages of motion and orientation and then, given enough data, can extrapolate to create 3-dimensional atomic-level movies of proteins in action. In effect, these new algorithms can show how proteins perform key biological functions, such as opening and closing channels to adjust the concentrations of key molecules in a cell.

The advent of these sophisticated data analysis tools is accelerating the pace of research. It took several decades to learn how to obtain 3-dimensional atomic-level pictures of static proteins, for example, but only another decade to go from still pictures to 3-D movies of proteins in action. However, the required database for a given protein needs to contain a million images or more. That's why protein researchers are increasingly making use of the X-ray free electron laser at DOE's SLAC National Accelerator Laboratory and similar facilities in Europe and Asia. These facilities provide powerful, ultra-short X-ray pulses and can take a billion separate images in the course of an experiment. The combination of abundant data and artificial intelligence algorithms are helping researchers develop better ways to combat the Covid pandemic and to understand other biological processes—even to predict protein structures based on their amino acid sequence. Moreover, the impact of powerful artificial intelligence algorithms is not confined to biology. Propelled by large databases and more powerful computers, data-driven research is likely to have an impact on many areas of science, as well as on commerce, in coming years.

Cryo-electron microscopes, such as the one shown here, are the most powerful in the world because they capture images with electrons, not light. Samples are frozen in a super-cooled container (inset).
(CREDIT: LAWRENCE BERKELEY NATIONAL LABORATORY)

Strategy: *Interplay among basic research, use-inspired research, applied research and industrial research*

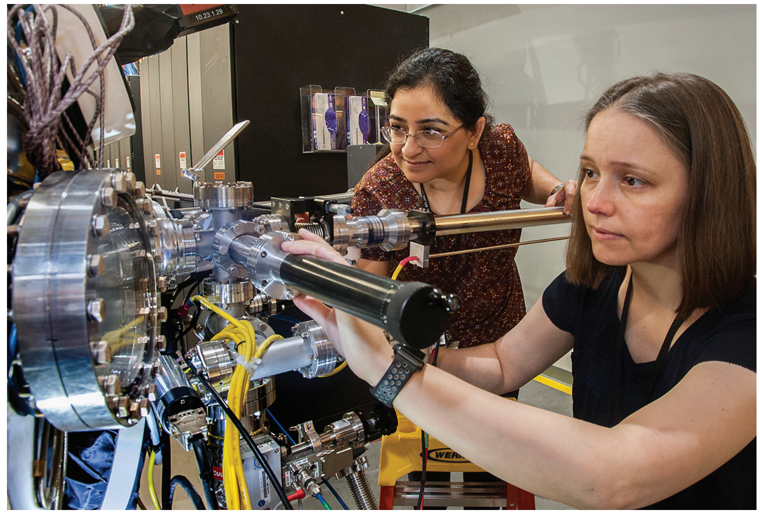
The words often used to describe the motivations for different sectors of research activities do not do justice to the subtle differences, and more importantly, the constructive interconnections, among those sectors. Industrial research depends on advances in basic scientific knowledge that industry itself no longer devotes much time or resources to develop. Basic science is often stimulated in unanticipated ways by problems encountered in its application to technology, and enabled by advanced tools from new technology developments.

This richer, more complete context used to exist in companies such as Bell Laboratories, IBM, GE, DuPont and others. Each of these companies created a research ecosystem that produced both Nobel Prize laureates and important commercial products, from the transistor and the laser to nylon and other polymers and many other important technologies. The point is that industry used to do basic research in an environment surrounded by scientists and engineers all along the spectrum from fundamental science to applied technology. There were many essential, non-Nobel actors involved in the post-discovery phase of these developments.

For that productive kind of research environment to be recaptured, better integration between basic and applied research will be necessary. In the context of research supported by the Department of Energy, an agency with an overarching mission, this report suggests that efforts to remove artificial barriers along the research spectrum from basic to applied could be useful. This view was supported in numerous consultations carried out during this study.

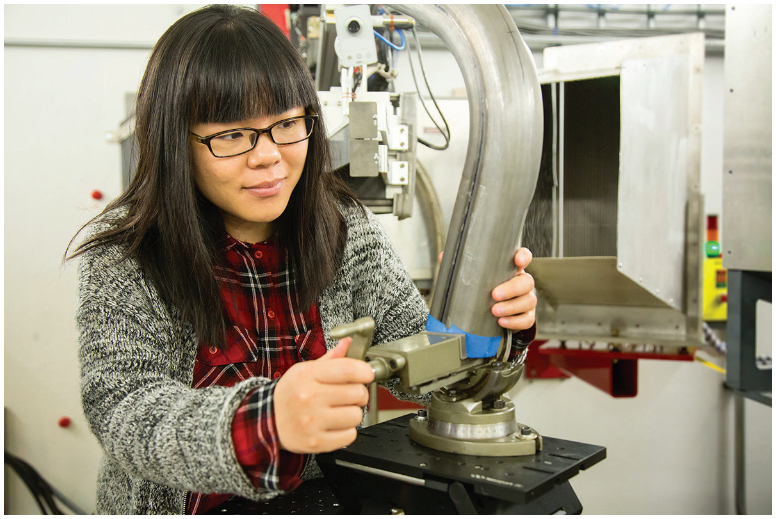
Recommendations. One way for the Office of Basic Energy Sciences to impact applied/industrial research is through its advanced research facilities, which offer tools to characterize materials and can be used for any research. That Office has already started to enhance connections with industrial research. One example is the recent BRN for Transformative Manufacturing.[13] Another example is sponsorship of industrial workshops at the user facilities, which has already begun to happen. This report includes a good example of an advanced research facility providing valuable access to a start-up company (see Box 2.1. Building a Better Battery). All the facilities have tried, to different degrees, to be better engaged with industry. It is not clear whether such activities are included in the triennial review of each facility, but that might be constructively examined. Similarly a review of whether staff scientists at such facilities have sufficient incentives to work with industrial researchers might be useful. Different national laboratories are managed in different ways. But if the Office of Basic Energy Sciences were to endorse industrial interaction more strongly, each advanced research facility might then be able to figure out how to accomplish this in their own way.

One of the priority research directions identified in the recent BRN for Transformative Manufac-



A Brookhaven National Laboratory staff scientist and a visiting researcher mount a material sample to measure its electronic structure with the laboratory's X-ray synchrotron. (CREDIT: BROOKHAVEN NATIONAL LABORATORY)

13. www.science.osti.gov/-/media/bes/besac/pdf/201907/900_Horton_-ransformative_Manufacturing_BRN_201907.pdf



Lu Huang, an industrial research engineer with United States Steel Corporation, prepares a light-weight high-strength steel component for neutron research at Oak Ridge National Laboratory's Spallation Neutron Source. (CREDIT: GENEVIEVE MARTIN/ORNL)

turing workshop is *in situ/operando* characterization under typical materials use and processing conditions, for which the advanced research facilities will play a particularly important role. To enable such research, facility scientists and researchers from academia and industry will have to work together. Moreover, as the instrumentation at advanced research facilities becomes more and more sophisticated, users of these facilities will have to work with knowledgeable staff scientists to make good use of it. Yet at present, it seems difficult to keep top talent at the research facilities. (See Box 3.5, Catalyzing a U.S. Manufacturing Revolution.) As discussed in the previous section, a more balanced approach to staff scientist activities that includes both user support and developing new capabilities for science seems worth considering.

Basic research is often focused on model materials/systems (often described as "proof of concept/principle") but applying them to real-world materials/systems is far from trivial. This is one of the issues the BRN for Transformative Manufacturing workshop begins to address under the topics of "system integration" and "scale-up". The Office of Basic Energy Sciences could consider involving applied/industrial researchers from an early stage, to enhance the ability of basic research initiatives to impact applied research. It is also important to be aware that problems of scale-up, kinetics and dynamics that are necessary for practical implementation may also give rise to new fundamental research problems. Better integration across the spectrum of basic, use-inspired, applied and industrial research could thus be highly beneficial for all parts of the spectrum. Several of the consultations for this report have pointed to opportunities for cooperation among DOE programs within and outside of the Office of Basic Energy Sciences.

BOX 3.5. **CATALYZING A U.S. MANUFACTURING REVOLUTION**

The key role of staff scientists at DOE advanced research facilities

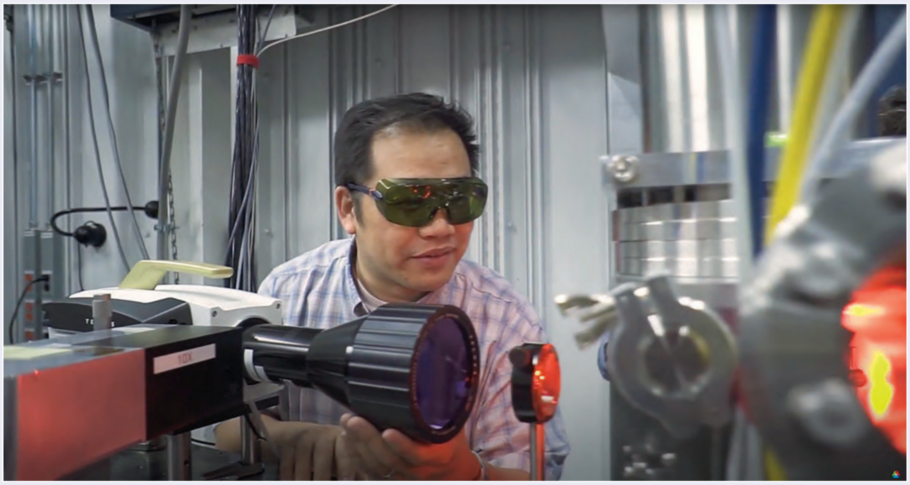
Our economy depends on precisely-shaped metal parts for aircraft engines, for implanted knee replacements, and many other purposes. Traditionally these have been manufactured by subtractive methods--cutting them out of a larger block of metal. The rise of additive manufacturing methods—for example, using a laser beam to melt metallic powder and build up the desired part layer by layer—promises both lower costs (by using less material) and the ability to create novel, more efficient shapes. Moreover, additive manufacturing (also called 3-D printing) does not require huge factories, so that parts can be created on demand, close to where they are needed, and can be easily customized to suit a particular application.

One obstacle to widespread use, however, has been that the laser fusion process commonly used to melt the powder can result in tiny gas bubbles that leave a void or defect in the finished product, which can lead to cracking—unacceptable for critical parts such as engine components. A breakthrough came last year when scientists at Carnegie Mellon University, the University of Virginia, and the U.S. Department of Energy's Argonne National Laboratory used the intense X-rays of the laboratory's synchrotron to study the laser fusion process in detail. They found that when the laser path over the powder creates a certain focused intensity, it is powerful enough to boil away the melted powder, creating a deep and highly fluctuating cavity that leads to voids. Moreover, the research provides a way to predict when such conditions will occur, potentially enabling manufacturers to adjust the laser settings in their manufacturing process so as to reliably create defect-free products and to speed up the additive process.

One major manufacturer that has already made the shift to additive manufacturing is GE Aviation. It makes fuel nozzle tips for turbofan jet engines at its plant in Auburn, Alabama.

These tips are complex structures that have passages for fuel and air and that would otherwise require connecting together 20 separate castings or sheet metal parts. At present, these parts are carefully inspected to eliminate any with defects, but the goal is to get a good part every time, regardless of the printer or batch of metal powder used. GE and other major manufacturers have done their own studies of the laser fusion process at the Argonne X-ray facility, but the story behind that unique capability starts much earlier.

Typically, the fundamental research behind a technological innovation precedes it by a decade or more. But additive manufacturing has evolved so quickly that both processes have happened in parallel. A key figure in the research, and a co-principal author on the breakthrough research described above, is Tao Sun. He was born in China, came to the U.S. for graduate studies in materials science and engineering, joined the Argonne laboratory in 2010, and was promoted to staff scientist in 2012. He became intrigued by the potential of additive manufacturing, and in collaboration with others built an X-ray beamline instrument to study it: in effect, a manufacturing simulator combining an X-ray probe, a high-power scanning laser, and specialized detectors including high-speed X-ray and infrared cameras. It produced thousands of images—in effect, movies—of the laser fusion process. Sun's early experiments created a lot of interest both from industry and from academic scientists, and demand to use the facility intensified so much that Sun had little time to pursue his own research. He eventually left Argonne in 2019 for a faculty position at the University of Virginia, where he is continuing to study the laser fusion process as well as many other additive processes in several different metal alloys of industrial interest, as well as exploring the use of artificial intelligence tools to automate the analysis of the data generated by the experiments.



Tao Sun in the beamline facility used for laser fusion studies that he helped to create at Argonne National Laboratory to improve additive manufacturing techniques. (CREDIT: ARGONNE NATIONAL LABORATORY)

CONCLUSIONS

The overall conclusion of this study is that the historical leadership position of the U.S. in basic scientific research of interest to DOE's Office of Basic Energy Sciences is eroding. The long-term consequences of this trend will be fewer innovations in the pipeline for future technology.

A major factor in the diminishment of U.S. leadership in basic science is the substantial investment in fundamental research by other countries in the past decade. That investment is paying dividends, based on the impact of research based in the EU and in Asia, especially China, in the areas selected for study.

One area of leadership that has persisted in the U.S. is advanced research facilities, including X-ray synchrotrons and free electron lasers, neutron sources, and electron microscopy. This leadership is a consequence of strategic planning and investment by the Office of Basic Energy Sciences.

On the other hand, development of small and mid-scale instrumentation in individual laboratories that often yields new technologies for commercial use is under pressure. These efforts, generally lower in profile, have historically led to new methods that are widely applied throughout society.

Investment in talent development and retention is also critical to future success in fundamental science and in technology. The U.S. was long considered an essential destination for career development of scientists; however, this is no longer the case. Opportunities and sustainable career paths of scientists are needed to slow or reverse this trend.

Finally, acceleration of technology development from basic science would be desirable. Basic science is the "seed corn" of innovation, but translation of fundamental work into an application generally requires decades of work, in part, because of the separations between fundamental and use-inspired work and between academic and industrial research. Better integration of fundamental and applied sciences has the potential to significantly shorten the time from discovery to application.

APPENDIX
METHODOLOGY AND RESULTS FOR STRATEGIC AREAS

Background

This appendix describes in greater detail the methodology and results regarding the charge to identify and benchmark areas of strategic importance to BES.

As a first step, the sub-committee reviewed previously-published literature, including reports on the status of U.S. competitiveness,[1] and a National Academy of Sciences (NAS) report on how to conduct international benchmarking studies.[2]

A key finding of the NAS report is that it is feasible to benchmark U.S. performance through "the establishment of independent panels consisting of researchers in the field" including some individuals who are "outstanding foreign scientists in the field." These field experts are "best qualified to appraise the quality of its researchers, identify the most promising advances, project the status of the field into the future, pinpoint locations where the most promising ideas are emerging, describe where the best new scientific talent chooses to work, judge the comparative quality of research facilities and human resources."[2] The NAS report further suggested that a "virtual congress" could be an efficient and credible way to evaluate fields. The meaning of "virtual congress" is that the field-experts "organize" a conference, identifying an international list of top speakers to invite, although the conference does not actually take place. Other activities cited as useful by the NAS report include citation and journal-publication analysis, quantitative data analysis (for example, number of graduate students, degrees, and employment status), and prize analysis.

Areas of Strategic Importance: Methodology and Results

To help select areas of strategic importance to BES, the committee started by reviewing all Basic Research Needs (BRN) documents[3] from the last ten years. The rationale for reviewing these documents is that, collectively, they comprehensively describe BES priorities. After careful deliberation on the strategic value to BES, a subset of BRN reports were selected and grouped into five areas (see Table A1). A panel of two experts, made up of sub-committee members, was assigned to each area.

The panels then conducted a study of the areas, which included discussions with experts in the areas including the chairs who wrote the BRN reports and the panel's own expertise in the areas. Sub-areas were identified and the current and future U.S. leadership position in each sub-area was assessed, based on the expert judgment of the panel and their consultants. The current and future leadership were assessed based on a 1–3 scale (see Table A2). The results of this assessment were used to create benchmarking tables.

1. *The Perils of Complacency, America at a Tipping Point in Science and Engineering*, American Academy of Arts and Sciences, 2020

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

3. www.science.osti.gov/bes/Community-Resources/Reports

TABLE A1. **Strategic Areas and Associated BRN Reports**

AREAS	BRN REPORTS RELEVANT TO THE AREA
Quantum information Science	BES Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences (2017) BES Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems (2017)
Science for energy	Roundtable on Liquid Solar Fuels (2019) BRN for Next Generation Electrical Energy Storage (2017) BRN for Synthesis Science for Energy Technologies (2016) BESAC Report on Science for Energy Technology (2010) BRN for Energy and Water (2017) BES Roundtable on Sustainable Ammonia Synthesis – Exploring the scientific challenges (2016)
Matter for energy and information	BRN for Microelectronics (2018) BES Roundtable on Neuromorphic Computing – From Materials Research to Systems Architecture (2015) BESAC Report on From Quanta to the Continuum: Opportunities for Mesoscale Science (2012) BES report on Computational Materials Science and Chemistry (2010)
Industrially-relevant science for sustainability	BRN Workshop on Transformative Manufacturing (2020) BES Roundtable on Chemical Upcycling of Polymers (2019) BRN for Catalysis Science to Transform Energy Technologies (2017) BRN on Quantum Materials for Energy Relevant Technology (2016) BRN for Carbon Capture: Beyond 2020 (2010)
Advanced research facilities	BES Roundtable on Opportunities for Basic Research at the Frontiers of XFEL Ultrafast Science (2017) BRN for Innovation and Discovery of Transformative Experimental Tools (2016) The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility Future of Electron Scattering and Diffraction (2014) BES Workshop On Future Electron Sources (2016)

TABLE A2. **Rating Scale for Current and Future U.S. Leadership**

CURRENT U.S. POSITION IN THIS FIELD INTERNATIONALLY	LIKELY FUTURE (5–10 YEARS) U.S. POSITION IN THIS FIELD
● 1 – Forefront	● 1 – Gaining/extending
● 2 – Among world leaders	● 2 – Maintaining
● 3 – Behind world leaders	● 3 – Losing potential

TABLE A3. **Quantum Information Science Benchmarking Table**

QUANTUM INFORMATION SCIENCE SUB-AREAS	CURRENT 1	CURRENT 2	CURRENT 3	FUTURE 1	FUTURE 2	FUTURE 3
QIS: Experiments		🟡			🟡	
QIS: Theory	🟢			🟢		
QIS: Bridging experiment and theory (compilation, software, etc)	🟢				🟡	

Note: The moderate discrepancy between results in this ranking in this table—derived from discussions with experts who are most connected with U.S. and EU projects—and the citation data (plotted below) is related to the different methodologies employed: each method can have inherent geographic bias ("home field advantage"). The citation data would advantage the region with more papers (e.g., Asia). A weighting factor should be considered when comparing the relative strength of various regions. However, the more systematic year over year changes in the citation data (below) do reflect the trends of the field.

TABLE A4. **Science for Energy Applications Benchmarking Tables**

NEXT GENERATION ENERGY STORAGE	CURRENT 1	CURRENT 2	CURRENT 3	FUTURE 1	FUTURE 2	FUTURE 3
THRUST 1. Tune Functionality of Materials and Chemistries to Enable Holistic Design for Energy Storage						
1a: Achieve simultaneous high power & high energy	🟢				🟡	
1b: Develop multifunctional solid electrolytes that enable safe solid-state batteries		🟡			🟡	🔴
THRUST 2. Link Complex Electronic, Electrochemical, and Physical Phenomena Across Time and Space						
2a: Create state-of-the-art modeling techniques and characterization tools		🟡			🟡	🔴
THRUST 3. Control and Exploit the Complex Interphase Region Formed at Dynamic Interfaces						
3a: Unravel interfacial complexity through in situ and operando characterization and theory		🟡			🟡	🔴
3b: Design solid-electrolyte interphase (SEI) for function	🟢				🟡	
THRUST 4. Revolutionize Energy Storage Performance through Innovative Assemblies of Matter						
4a: Design and synthesize new mesoscale architectures	🟢				🟡	
THRUST 5. Promote Self-healing & Eliminate Detrimental Chemistries to Extend Lifetime & Improve Safety						
5a: Conduct multi-modal in situ experiments to quantify degradation and failure		🟡			🟡	🔴

LIQUID SOLAR FUELS	CURRENT 1	CURRENT 2	CURRENT 3	FUTURE 1	FUTURE 2	FUTURE 3
Artificial photosynthesis	🟢				🟡	
Electrochemistry (materials/catalysis)		🟡			🟡	

TABLE A5. Innovative Use of Matter for Energy and Information Benchmarking Table

	CURRENT			FUTURE		
INNOVATIVE USE OF MATTER FOR ENERGY AND INFORMATION	1	2	3	1	2	3
Quantum materials		● (yellow)				
Nanoscience	● (green)			● (green)		
Neuromorphic computing	● (green)				● (yellow)	

TABLE A6. Industrially Relevant Science for Sustainability Benchmarking Table

	CURRENT			FUTURE		
INDUSTRIALLY RELEVANT SCIENCE FOR SUSTAINABILITY	1	2	3	1	2	3
Chemical upcycling of polymers		● (yellow)		● (green)		
Catalysis science to transform energy technologies		● (yellow)			● (yellow)	
Carbon capture			● (red)			● (red)

TABLE A7. Advanced Tools (Cross-Cutting) Benchmarking Table

	CURRENT			FUTURE		
FACILITIES	1	2	3	1	2	3
Neutron scattering		● (yellow)	● (red)		● (yellow)	● (red)
Isotope production	● (green)			● (green)		
Materials irradiation	● (green)				● (yellow)	
X-ray free electron laser (XFEL)	● (green)				● (yellow)	
Electron microscopy science	● (green)			● (green)		
Electron microscopy facilities			● (red)			● (red)
Ultrafast electron scattering/diffraction		● (yellow)				● (red)

Deep-dive Sub-areas. Conference and Citation/Literature Methodology and Results

Based on the assessments (as summarized in the preceding benchmarking tables), and again consulting the judgment of area experts, key sub-areas were selected for "deep dive" study (Table A8). Two primary methodologies were used to analyze the selected sub-areas, a conference analysis and citation/literature analysis.

TABLE A8. Five Areas Identified as Critical to the BES Mission with Selected Subareas

	AREAS	SUB-AREAS
1	**Quantum Information Science**	Quantum computation, quantum communication, quantum simulation, quantum sensing
2	**Science for Energy Applications**	Membranes, interfaces, energy storage, sustainable fuels
3	**Matter for Energy and Information**	Quantum materials, mesoscience, nanoscience, neuromorphic computing
4	**Industrially-Relevant Science for Sustainability**	Chemical upcycling of polymers, electrocatalysis, carbon capture, transformative manufacturing
5	**Advanced Research Facilities**	Neutron sources, synchrotron and free electron laser X-ray sources, electron microscopy

Conference Analysis

Methodology

Following a key recommendation of the NAS report,[4] the sub-committee decided to start the analysis using an analysis of conferences, which is a modified "virtual congress" methodology from the NAS report. By virtual congress, the authors of the report meant that area experts should do the work to organize an international conference on the selected area, including to select invited speakers that would be invited. Although the conference would never actually take place (hence, "virtual"), the nationalities of the invited speakers would serve as a good benchmarking indication of international leadership in the area. This method was experimentally validated by the NAS authors.

For this report, a slightly modified methodology based on the virtual congress concept was used. Instead of designing "virtual" conferences from scratch, the area experts selected relevant international conferences that actually occurred (or were organized, even if they did not actually occur because of Covid-19) over the past few years. This modified method makes sense, because this kind of conference information is now widely and publicly available on the internet, a condition which probably did not exist when the NAS report was written. Using this method, a much larger number of conferences and invited speakers were able to be analyzed than would have been possible only using the virtual congress method.

While conducting the conference study, it became clear that there is a very high risk of "home field advantage" bias: there are often more invited speakers from the conference host-country than might normally be invited. This seems quite natural, as there could be many reasons why invited speakers may not be willing or able to travel internationally for a particular conference. In an effort to reduce this bias, the committee devised two ways to count the invited speakers. In the first way, the "Inclusive Count," all invited speakers were counted at all conferences, which does not do anything to prevent the bias. In the second way, the "Exclusive Count," speakers from the host country are *excluded* from the count, unless there was clear evidence that the speaker selection committee was made up of an international group with less than half of the members from the host country (as is typically the case for Gordon conferences, for example). The exclusion was extended across the EU as a "bloc," so for example a speaker from Germany would be excluded from the count if the conference occurred in any EU country. For the purposes of this study, UK and Israel were included as part of the EU ("Brexit" had not yet had an effect, Israel is highly integrated in EU funding). Russia was not included as an EU nation. The data showed that the exclusive count significantly reduced the "home field" bias, although it is not known if the method fully eliminated the bias.

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4. Committee on Science Engineering and Public Policy, *Experiments in International Benchmarking of U.S. Research Fields* (Washington, D.C.: National Academies Press, 2000), www.doi.org/10.17226/9784

Quantum Information Science Conference Results

Conferences on quantum information science, results from 21 conferences, with a total of 683 invited speakers from 31 nations

TABLE A9. Conferences on Quantum Information Science

Jan 14–18, 2019: 22nd Annual Conference on Quantum Information Processing (QIP 2019), Boulder, United States of America *Note: All speakers are considered invited because the conference committee selects submissions competitively*
Feb 18–22, 2019: European Quantum Technologies Conference 2019 (EQTC2019), Grenoble, France
Feb 25–Mar 1, 2019: Workshop on Ubiquitous Quantum Physics: the New Quantum Revolution, Trieste, Italy
Mar 4–8, 2019: March Meeting of the American Physical Society, Boston, United States of America
Apr 4–6, 2019: Quantum Information and Measurement V: Quantum Technologies (QIM2019), Rome, Italy
GRC: Jun 2–7, 2019: Quantum Sensing Applications in Metrology and Imaging Conference, Hong Kong, China
Jun 3–7, 2019: Fourteenth Conference on the Theory of Quantum Computation, Communication, and Cryptography (TQC 2019), College Park, United States of America
Jun 24–28, 2019: 2019 Adiabatic Quantum Computing Conference (AQC 2019), Innsbruck, Austria
Jul 29–Aug 2, 2019: 5th International Conference on Quantum Error Correction (QEC19), London, United Kingdom
Aug 19–23, 2019: 19th Asian Quantum Information Science Conference (AQIS'19), Seoul, Korea
Sep 15–20, 2019: International Conference on Emerging Quantum Technology, Hefei, China
Dec 9–13, 2019: International Conference on Quantum Metrology and Sensing (IQuMS 2019), Paris, France
Feb 4–8, 2019: SFB-FoQuS International Conference, Innsbruck, Austria
Apr 8–10, 2019: Quantum Computing Theory in Practice, Bristol, United Kingdom
May 27–31, 2019: 50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, Milwaukee, United States of America
Jun 23–28, 2019: Symposium on Diamond and Single Photon Emitters (ICMAT'19), Singapore
Aug 26–30, 2019: Conference on Quantum Information and Quantum Control (CQIQC-VIII), Toronto, Canada
11th QIP 2007, New Delhi
16th QIP 2013, Tsinghua University
17th QIP 2014, Barcelona

TABLE A10. Quantum Information Science Conference Results

REGION/ COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
EU	336	232
Asia	66	46
U.S.	210	140
Canada	45	40
Australia	22	22
Iran	2	2
South Africa	1	1
Russia	1	1

Science for Energy Applications Conference Results

Membranes and Interfaces

Conferences on membranes and interfaces, results from 10 conferences, with a total of 572 invited speakers from 33 nations

TABLE A11. Conferences on Membranes and Interface

GRC 2018: Translating Molecular Scale Discoveries to Commercial-Scale Membrane Operations
GRC: 2016: Debates and Controversies in the Field of Membranes
International Conference on Membranes and Membrane Processes, 2020
The 2nd International Conference on Energy-Efficient Separation (MDPI[1]) 2019
4th International Conferences on Desalination Using Membrane Technology (Elsevier) 2020
MEMTEK International Symposium on Membrane Technologies and Separations 2019
MRS Spring meeting 2017 https://www.mrs.org/spring2017
MRS Spring meeting 2018
MRS Spring Meeting 2019 https://www.mrs.org/spring2019
https://www.mrs.org/fall2019
MRS Fall Meeting 2017
Symposium on Membranes MRS Spring 2021 *(virtual meeting)*
E-MRS 2021, Spring

Sustainable Fuels

Conferences on sustainable fuels, results from 9 conferences, with a total of 288 invited speakers from 29 nations

TABLE A12. Membranes and Interfaces Conference Results

COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
U.S.	287	160
EU	116	93
China	41	41
Japan	21	21
South Korea	19	19
Singapore	12	12
Australia	54	7
Saudi Arabia	6	6
Malaysia	3	3
India	3	3
Canada	2	2
Taiwan	2	2
UAE	2	2
South Africa	1	1
Qatar	1	1
Brazil	1	1
Turkey	1	0

TABLE A13. Conferences on Sustainable Fuels

GRC: Electrochemical Interfaces in Energy Conversion and Storage, The Hong Kong University of Science and Technology, Hong Kong, China, 2020
GRC: Storing Solar Energy in Chemical Bonds: From Theory and Catalysis to Devices and Engineering, Ventura, CA, 2018
GRC: Green Chemistry Chemical Sciences Driving Sustainability, July 26–31, 2020, Rey Don Jaime Grand Hotel, Castelldefels, Spain
GRC: Carbon capture, utilization and storage 2021, New Hampshire U.S.
GRC: Electrochemistry January 2020—Bridging Scales in Electrochemical Materials and Methods Applied to Organic and Inorganic Chemistry, Catalysis, Energy and Biology, Ventura CA
International solar fuels conference, Hiroshima, Japan, 2019 http://photoenergy-conv.net/ICARP2019/
International Society of Electrochemistry 2019 https://www.ise-online.org/ise-conferences/annmeet/reports/ann_meeting_report_2019.pdf South Africa
2018 — https://www.ise-online.org/ise-conferences/annmeet/folder/69th_Annual_meeting-BoA.pdf Italy
2017 — https://www.ise-online.org/ise-conferences/annmeet/folder/68-Annual-program.pdf USA

TABLE A14. Sustainable Fuels Conference Results

REGION/ COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
EU	105	102
Asia	33	24
U.S.	128	125
Australia	5	5
Canada	10	10
Chile	3	3
Ethiopia	1	1
Qatar	1	1
Russia	1	1
South Africa	1	0

Innovative Use of Matter for Energy and Information

Quantum Materials

Conferences on quantum materials, results from 11 conferences, with a total of 366 invited speakers from 30 nations

TABLE A15. Conferences on Quantum Materials

CEMS/Riken Emergent Quantum Materials, Tokyo, 2019
Gordon Research Conf. Topological and Correlated Matter, Hong Kong, 2019
Gordon Research Conference Superconductivity, Switzerland, 2019
Gordon Research Seminar Superconductivity, Switzerland, 2019
Graphene and 2DM Virtual Conference, Spain, 2020
International Conf on Low Energy Electrodynamics in Solids, USA, 2020
International Conference on Low Temperature Physics, Japan, 2020
International Conference on Strongly Correlated Electron Systems, Brazil, 2020
Spectroscopies in Novel Superconductors, Tokyo, 2019
Topological Matter School, San Sebastian, Spain, 2020 *(cancelled)*

TABLE A16. Quantum Materials Conference Results

REGION/ COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
EU	146	103
Asia	74	44
U.S.	109	92
Canada	16	16
Brazil	16	2
Australia	1	1
Russia	1	1
Argentina	2	2
New Zealand	1	1

Quantum Materials, *continued*

Conferences on mesoscopics/nanoscience, results from 6 conferences, with a total of 231 invited speakers from 17 nations

TABLE A17. Conferences on Mesoscopics/Nanoscience

GRC Computational Materials Science and Engineering Comparing Theories, Algorithms and Computation Protocols in Materials Science and Engineering, August 2–7, 2020, Grand Summit Hotel at Sunday River, Newry, ME
GRC Computational Chemistry Multiscale Modeling of Complex Systems: Methods and Applications, July 19–24, 2020, Rey Don Jaime Grand Hotel, Castelldefels, Spain
GRC Energetic Materials The Confuence of Science-Based and Machine Learning Approaches in Energetic Materials Research, May 31–June 5, 2020 • Grand Summit Hotel at Sunday River, Newry, ME
GRC: Fundamental Mechanisms of Ordering from the Atomic to the Mesoscale, June 28–July 3, 2015
GRC: Mechanistic Understanding of the Growth and Assembly of Ordered Materials 2019, Manchester, NH
GRC: Mechanistic Understanding of the Growth and Assembly of Ordered Materials 2017, University of New England

TABLE A18. Mesoscopics/Nanoscience Conference Results

COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
U.S.	150	150
EU	67	67
Canada	4	4
Japan	3	3
Australia	3	3
Saudi Arabia	2	2
Singapore	1	1
China	1	1

Industrially Relevant Science for Sustainability

Sustainable Catalysis

Conferences on sustainable catalysis, results from 10 conferences, with a total of 195 invited speakers from 22 nations

TABLE A19. Conferences on Sustainable Catalysis

GRC Catalysis-Conference 2018
GRC Catalysis-Conference 2016
GRC Catalysis-Conference 2014
NAM 2019 US
NAM 2017 US
NAM 2015 US
NAM 2013 US
ISHHC19
ISHHC XIII (2007)
ISHHC-16 (2013)

TABLE A20. Sustainable Catalysis Conference Results

COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
U.S.	126	73
EU	54	51
China	4	4
Japan	7	2
Canada	2	2
Brazil	1	1
Australia	1	1

Advanced Tools

Neutron Scattering

Conferences on neutron scattering, results from 7 conferences, with a total of 169 invited speakers from 19 nations

TABLE A21. Conferences on Neutron Scattering

ACNS 2020, USA
European Conference on Neutron Scattering (ECNS) June 30–July 5, 2019, St. Petersburg, Russia *(next meeting in 2021)*
Gordon Research Conference on Neutron Scattering (May 5–10, 2019), Hong Kong *(also held 2015 and 2017)*
German Neutron Scattering Conference (DN2020) Dec. 9–10, 2020, Munich, Germany
2021 Annual MLZ Conference: Neutrons for Life Sciences; June 8–11, 2021
SXNS16-16th International Conference on Surface X-ray and Neutron Scattering, 2020
ICNS 2021- International Conference on Neutron Scattering, July 4–8, 2021, Buenos Aires, Argentina

TABLE A22. Neutron Scattering Conference Results

COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
EU	79	63
U.S.	49	14
Japan	8	8
Canada	4	4
Australia	2	2
Korea	1	1
India	1	1
Russia	18	0
China	7	0

Electron Microscopy

Conferences on electron microscopy, results from 4 conferences, with a total of 169 invited speakers from 21 nations

TABLE A23. Conferences on Electron Microscopy

International Federation of Microscopy Societies, International Microscopy Congress, Australia http://imc19.com/program/
MRS Symposium CM02: In Situ TEM Characterization of Dynamic Processes During Materials Synthesis and MRS Processing https://www.mrs.org/spring-2018-symposium-sessions-detail?code=CM02 *(considered international, invited speakers only)*
MRS 2017 Symposium CM4: In Situ Electron Microscopy of Dynamic Materials Phenomena https://www.mrs.org/spring2017/spring-2017-symposia/?code=CM4 *(considered international, invited only)*
MRS 2020 Symposium F.MT03—Frontiers of Imaging and Spectroscopy in Electron Microscopy https://www.mrs.org/meetings-events/fall-meetings-exhibits/2020-mrs-spring-and-fall-meeting/call-for-papers/call-for-papers-detail?code=F.MT03 *(considered international, invited speakers only)*

TABLE A24. Electron Microscopy Conference Results

REGION/ COUNTRY	INCLUSIVE COUNT	EXCLUSIVE COUNT
U.S.	62	62
EU	60	60
Asia	23	23
Canada	3	3
Australia	19	1
South Africa	1	1
Saudi Arabia	1	1

Citation/Literature Analysis

Methodology

The Scopus abstract and citation database was used for the literature search. Scopus is a source-neutral abstract and citation database curated by independent subject matter experts with over 25,100 source titles (over 23,452 peer-reviewed journals) from more than 5,000 international publishers. Scopus covers research output in the fields of science, technology, medicine, social science, and arts and humanities, and the Scopus database contains over 77.8 million records: over 71.2 million post-1969.

The search was divided into two phases for each sub-area, Phase 1 (to identify contributions by country/region based on keywords) and Phase 2 (to investigate the use of advanced tools and facilities as they cross-cut the sub-areas).

Phase 1 Methodology

Using lists of keywords generated by the committee (Scheme 1) the Scopus citation database was searched, limiting to the timeframe: 2010-2019. Additionally, the search results were limited to document types labeled "Articles" or "Conference Paper."

Searching "All Fields" resulted in a large number of irrelevant results. Therefore, the search fields were limited to the "Article title, Abstract, Keywords" to focus on the highly relevant results.

As part of cleaning the final data, duplicate records were removed. Any records that did not download properly or contained scrambled information were also removed, prior to determining Country and Region fields. To ensure the keywords returned appropriate papers, a random sample of papers from each of the areas were reviewed by area-experts from the committee. The "error" rate of papers that were not considered relevant was less than 10%.

SCHEME 1. KEYWORDS USED IN SCOPUS SEARCH STRINGS FOR THE VARIOUS SUB-AREAS

Quantum Information

{Quantum computation} OR {quantum control} OR {quantum error correction} OR {quantum information processing} OR {quantum metrology} OR {quantum sensing} OR {quantum communication}

Membranes

({"reverse osmosis membrane"} OR {nanofiltration membrane} OR {ultrafiltration membrane}) AND ({polymer} OR {metal-organic framework} OR {covalent organic framework} OR {porous} OR {microporous}) AND ({water} OR {energy} OR {gas separations} OR {ion separations} OR {selective})

Energy Storage

{Energy storage AND battery} OR {electrochemical energy storage} OR {energy storage AND rechargeable} OR {energy storage AND ion battery} OR {energy storage AND Battery charging time} OR {energy storage AND Battery energy density} OR {energy storage AND Battery power density} OR {energy storage AND Battery cycle lifetime} OR {energy storage AND Battery electrolyte} OR {energy storage AND separator} OR {energy storage AND Battery anode or battery negative electrode} OR {energy storage AND Battery cathode battery positive} OR {energy storage AND Flow battery}

Quantum Materials

{Bismuth-based superconductors} OR {Charge Density Wave} OR {Chern Insulator} OR {Chiral superconductivity} OR {Chiral transport} OR {Cooper Pair} OR {Correlated states} OR {Correlated insulator} OR {Cuprate superconductors} OR {d-wave} OR {Density Wave} OR {Dichalcogenide} OR {Dirac Semi metal} OR {Dirac Surface State} OR {Emergent phenomena} OR {Floquet-Bloch} OR {Fractional Quantum Hall} OR {Graphene} OR {Heavy Fermion} OR {High Tc superconductivity} OR {Insulator Metal Transition} OR {Iron-based superconductors} OR {Kondo} OR {Magic Angle} OR {Metal-Insulator transition} OR {Moire superlattice} OR {Mott Insulator} OR {Pnictide superconductors} OR {pseudogap} OR {Quantum Anomalous Hall} OR {Quantum Criticality} OR {Quantum Hall} OR {Quantum Spin Hall} OR {quasi particle} OR {RuCl3} OR {Spin density wave} OR {Strongly Correlated} OR {Superconducting} OR {Superconductivity} OR {Superconductor} OR {Topological Hall Effect} OR {Topological Insulator} OR {Topological Semimetal} OR {Transition metal dichalcogenide} OR {Twisted Bilayer Graphene} OR {Under-doped} OR {Van der Waals crystal} OR {Van der Waals heterostructure} OR {Weyl Semimetal}

Electrocatalysis and Polymer Upcycling

{Polymer upcycling} OR {Carbon capture} OR {CO2 OR carbon dioxide} OR {Circular chemical processing} OR {Circular economy} OR {Carbon dioxide reduction} OR {Catalysis for sustainability} OR {Electrocatalysis} OR {Renewable polymers} OR {Recyclability}

The data obtained using the Scopus search was further processed to identify the papers cited in the top *x* percentile for any given year, where *x* can be any number from "cited at least 1 time" to the top 1-percentile. To identify these papers, for each year, all papers worldwide are sorted by number of times they were cited. If N is the number of times the paper at the *x*th percentile was cited, pick all papers with N or more citations. This method prevents a possible "sort order" bias (ie, papers from Algeria are not accidentally picked more than papers from Zimbabwe).

The results were then plotted in various ways. The total number of citations for the U.S., EU, Asia and the next top-two nations (for total citations integrated over years) were plotted against year to show the trend in publication. This plot was made for various "top percentile" publications (top 20%, top 5% cited, etc). The same data were also converted to the world-wide percentage of total publications of a given percentile (not double-counting Asia and EU, obviously). On these plots, the raw data are shown as markers, and a slightly-smoothed "guide to the eye" line is shown. In a different style of graph, the top-18 nations, plus EU and Asia, were plotted for years 2000 and 2019 to provide a broader picture of the top producing countries/regions, just for a snapshot of years.

Phase 2 Methodology

The aim of this Phase was to analyze the dataset from phase 1 for facilities use; looking at the last 10 years of data (2010-19) using facilities found in the top 1% most highly cited papers. Determine the geographical location of facilities used (city, country, region), and methods of research used for the research in each article. The Phase 2 facilities list (Scheme 2) was used to search each article, to assist with identifying specific research methods.

The Phase 1 data was sorted by the times "Cited" column, and the top 1% of most highly cited articles. Using the DOI (Digital Object Identifier), a unique and permanent article identifier for each article, a search was conducted to find the full-text PDF files of all articles. Most of these articles were available from the publisher as Open Access, and were easily obtained via a search of the internet (specifically, searching Google Scholar was helpful). Remaining non-Open Access articles were obtained from subscription databases. Once all full-text files were collected they were deposited into one folder. Each article file was named using the DOI to ensure that matching the PDF files with the data records in the spreadsheet was easy to accomplish.

To ensure the searching was manageable, the full-text articles were broken down into smaller batches of ~20 files each. An index was created for each sub-set of files using Adobe Acrobat to quickly search across the set of 20 articles for the Phase 1 Keywords Search Strings and identify which files contained each of the keywords.[5] Through this systematic searching of each of the articles, the research methods were found and transferred to the spreadsheet, using the DOI/title of article to ensure data was being matched with the correct record in the spreadsheet. A significant amount of manually reading portions of the articles was also involved.

After the search was completed, a matrix was generated to cross the country where each paper was written with the country where facilities were used. Each row/column in the matrix is a country, but a row is also generated for "EU" and "Asia". When summing over row or column, the "EU" and "Asia" row are obviously not counted because that would result in countries being counted twice.

5. Learn more about creating PDF indexes online at https://helpx.adobe.com/acrobat/using/creating-pdf-indexes.html.

SCHEME 2. FACILITIES LIST

NORTH AMERICA

Canada

Canadian Light Source OR CLS OR Centre canadien de rayonnement synchrotron [at U Saskatchewan]

Canadian Centre for Electron Microscopy OR CCEM [at McMaster U]

USA

Argonne OR ANL

Advanced Photon Source OR APS

Argonne Leadership Computing Facility OR ALCF

Center for Nanoscale Materials OR CNM

Brookhaven OR BNL

National Synchrotron Light Source II OR NSLS-II

Center for Functional Nanomaterials OR CFN

Lawrence Berkeley OR LBNL OR LBL OR Berkeley Lab

Advanced Light Source OR ALS

National Energy Research Scientific Computing Center OR NERSC

Molecular Foundry

National Center for Electron Microscopy OR NCEM

National Institute of Standards and Technology OR NIST

Center for Neutron Research OR NCNR

Synchrotron Ultraviolet Radiation Facility OR SURF

Oak Ridge OR ORNL

Spallation Neutron Source OR SNS

High Flux Isotope Reactor OR HFIR

Leadership Computing Facility OR OLCF

Center for Nanophase Materials Sciences OR CNMS

Stanford Linear Accelerator Center OR SLAC

Linac Coherent Light Source OR LCLS

Synchrotron Radiation Lightsource OR SSRL

Cryo-electron Microscopy OR Cryo-EM OR S2C2

Cornell High Energy Synchrotron Source OR CHESS

Missouri Research Reactor Center OR MURR

Jefferson Laboratory Free Electron Laser OR Jlab OR Thomas Jefferson National Accelerator Facility OR TJNAF

Synchrotron Radiation Center OR SRC OR Tantalus [at Wisconsin]

Center for Advanced Microstructures and Devices OR CAMD [at LSU]

Center for Terahertz Science and Technology OR CTST [at UCSB]

Duke Free Electron Laser Laboratory OR DFELL [at Duke]

Keck Vanderbilt Free-electron Laser Center [at Vanderbilt]

LATIN AMERICA

Brazil

Laboratório Nacional de Luz Síncrotron OR Brazilian Synchrotron Light Laboratory OR LNLS OR Center of Research in Energy and Materials OR CNPEM OR Sirius

Mexico

Proyecto Sincrotrón Méxicano OR Mexican Synchrotron Project [at Hidalgo]

EUROPE, including UK

Denmark

ASTRID OR Centre for Storage Ring Facilities OR ISA

France

Institut Laue-Langevin OR ILL

Leon Brillouin Laboratory OR Laboratoire Léon Brillouin OR LLB OR Saclay Centre

Synchrotron Soleil

European Synchrotron Radiation Facility OR ESRF

Anneau de Collisions d'Orsay OR ACO

LURE OR Laboratoire pour l'Utilisation du Rayonnement Electromagnétique

Centre Laser Infrarouge d'Orsay OR CLIO OR Laboratoire de Chimie Physique OR LCP

Germany

Deutsches Elektronen-Synchrotron OR DESY OR German Electron Synchrotron OR DORIS OR Doppel-Ring-Speicher OR PETRA

European X-Ray Free-Electron Laser Facility OR European XFEL

(Juelich OR Jülich) Centre for Neutron Science OR JCNS

Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen OR Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons OR ER-C

Forschungsreaktor München II or FRM II OR Research Neutron Source Heinz Maier-Leibnitz OR Forschungs-Neutronenquelle Heinz Maier-Leibnitz

Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung OR BESSY OR Berlin Electron Storage Ring Society for Synchrotron Radiation OR Helmholtz-Zentrum Berlin

ANKA OR Karlsruhe Institute of Technology

Metrology Light Source OR MLS

DELTA

Italy

Frascati Synchrotron Radiation Collaboration OR Laboratori Nazionali di Frascati OR Solidi Roma

Synchrotron Radiation Facility OR Progetto Utilizzazione Luce di Sincrotrone OR PULS OR DAFNE ELETTRA OR FERMI

Netherlands

Free Electron Laser for Infrared eXperiments OR FELIX

Poland

Solaris

Spain

ALBA

Sweden

[under construction] European Spallation Source OR ESS

Max IV Laboratory

Switzerland

Paul Scherrer Institute OR PSI OR Swiss X-ray free-electron laser OR SwissFEL OR Swiss Light Source OR SLS OR SINQ spallation source OR SINQ neutron source

UK

Rutherford Appleton Laboratories (RAL) OR Harwell Campus OR Diamond Light Source OR ISIS Neutron and Muon Source [spinoff of Diamond Light Source]: Quantum Detectors Ltd

SCHEME 2. FACILITIES LIST, *continued*

SuperSTEM OR SuperSTEM Daresbury OR EPSRC National Research Facility for Advanced Electron Microscopy OR Daresbury

From ESTEEM-3 OR Enabling Science and Technology through European Electron Microscopy list of consortium members:

Austria: FELMI OR Institute for Electron Microscopy and Nanoanalysis OR Graz University of Technology OR TU Graz OR Technische Universitat Graz

Belgium: NanoMEGAS

France: CEMES-CNRS laboratory OR Centre d'Elaboration des Matériaux et d'Etudes Structurales

CNRS-LPS laboratory OR Laboratoire de Physique des Solides

Germany: Forschungszentrum Jülich

Germany: Max Planck Society OR MPG OR Stuttgart Center for Electron Microscopy OR StEM OR Max Planck Institute for Solid State Research OR MPI-FKF

Germany: Corrected Electron Optical Systems OR CEOS

Italy: Consiglio Nazionale delle Ricerche OR National Research Council OR CNR OR Institute for Microelectronic and Microsystems OR IMM

Belgium: Universiteit Antwerpen OR University of Antwerpen OR Electron Microscopy for Materials Science OR EMAT

Netherlands: DENSsolutions

Norway: Norwegian University of Science and Technology OR NTNU OR NORTEM OR Norges Teknisk-Naturvitenskapelige Universitet

Poland: International Centre for Electron Microscopy for Materials Science OR IC-EM OR AGH University of Science and Technology OR AGH-UST OR Akademia Gorniczo-Hutnicza

Slovenia: Jožef Stefan Institute OR JSI

Spain: University of Zaragoza OR UNIZAR OR Nanoscience Institute of Aragon OR INA

Spain: University of Cadiz OR UCA

Sweden: Chalmers tekniska hoegskola OR Chalmers University of Technology OR Chalmers Materials Analysis laboratory OR CMAL

Switzerland: Attolight

UK: Cambridge OR Oxford

ASIA

China

Shanghai Synchrotron Radiation Facility OR SSRF Shanghai XFEL OR X-ray Free Electron Laser

Beijing Synchrotron Radiation Facility OR BSRF

Beijing Electron–Positron Collider II OR BEPC II

National Synchrotron Radiation Laboratory OR NSRL [in Hefei]

India

Indus OR Raja Ramanna Centre for Advanced Technology

Japan

Super Photon ring-8 OR SPring-8 OR SPring-8 Angstrom Compact Free Electron Laser OR SACLA OR RIKEN OR HARIMA

Photon Factory OR PF OR High Energy Accelerator Research Organization OR KEK

Institute for Solid State Physics Neutron Scattering Laboratory OR ISSP OR NSL OR Japan Proton Accelerator Research Complex OR J-PARC

Institute for Nuclear Studies-Synchrotron Orbital Radiation OR INS-SOR

Yuichi Ikuhara OR Advanced Institute for Materials Research OR AIMR OR Nano Interface Technology Research Group

Kazu Suenaga OR National Institute for Advanced Industrial Science and Technology OR AIST

Hiroshima Synchrotron Radiation Center OR HSRC

Institute of Free Electron Laser OR iFEL [at Osaka U]

IR FEL Research Center OR FELSUT OR VSX Light Source [at Tokyo U]

Medical Synchrotron Radiation Facility [at National Institute of Radiological Sciences, Chiba]

Nagoya University Small Synchrotron Radiation Facility OR NSSR Photonics Research Institute [at Tsukuba Science City]

Saga Light Source OR SAGA-LS

Ultraviolet Synchrotron Orbital Radiation Facility OR UVSOR [at National Institutes of Natural Sciences, Okazaki]

Jordan

Synchrotron-Light for Experimental Science and Applications in the Middle East OR SESAME

Russian Federation

Kurchatov Synchrotron Radiation Source1 OR SIBIR-1 OR SIBIR-2 OR Kurchatov Institute

Dubna Electron Synchrotron OR DELSY Siberian Synchrotron Radiation Centre OR SSRC OR Budker Institute of Nuclear Physics

Technical Storage Ring Complex OR TNK OR FV Lukin Institute

Singapore

Singapore Synchrotron Light Source OR SSLS

South Korea

Pohang Accelerator Laboratory X-ray Free Electron Laser OR PAL-XFEL

Taiwan

Taiwan Photon Source OR TPS OR Taiwan Light Source OR TLS OR National Synchrotron Radiation Research Center OR NSRRC

Thailand

Synchrotron Light Research Institute OR SLRI

OCEANIA

Australia

Australian Centre for Neutron Scattering OR Bragg Institute OR Australia's Nuclear Science and Technology Organisation OR ANSTO

Monash Centre for Electron Microscopy OR MCEM

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1. https://en.wikipedia.org/wiki/Kurchatov_Center_for_Synchrotron_Radiation_and_Nanotechnology

QUANTUM INFORMATION RESULTS

Note: Raw data are shown as markers. Solid lines have been smoothed to serve as guides to the eye.

Figure A1.A

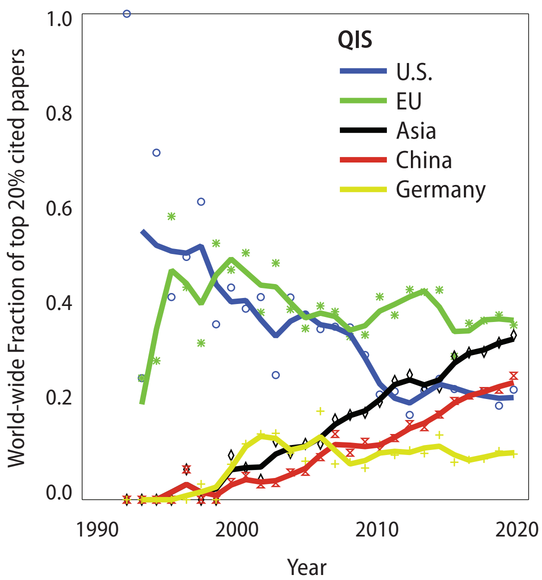


Figure A1.B

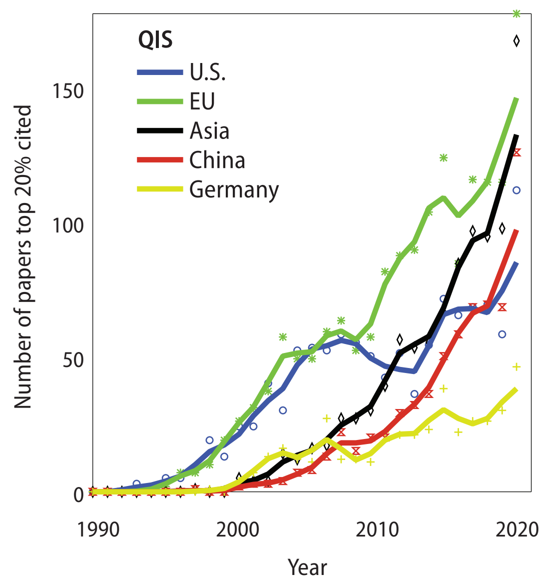


Figure A1.C

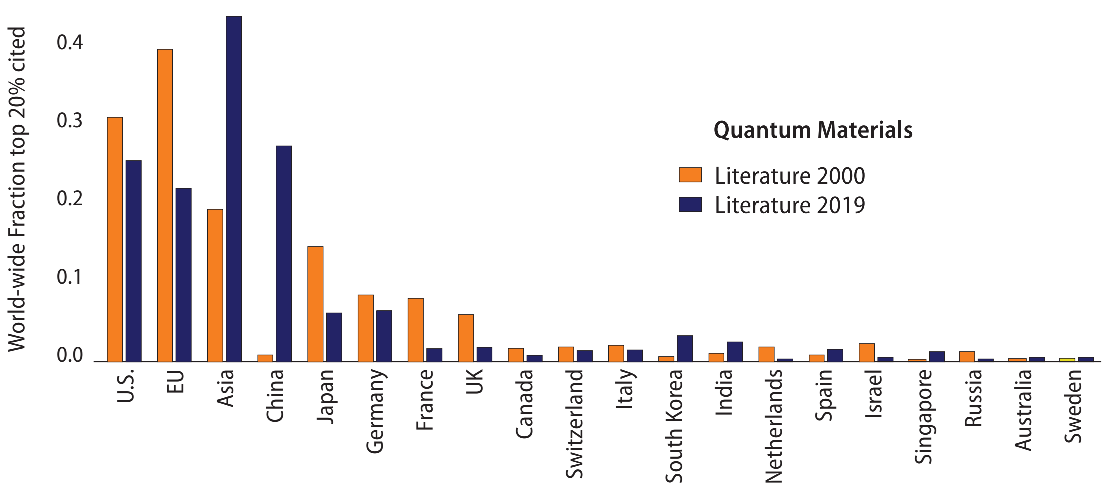
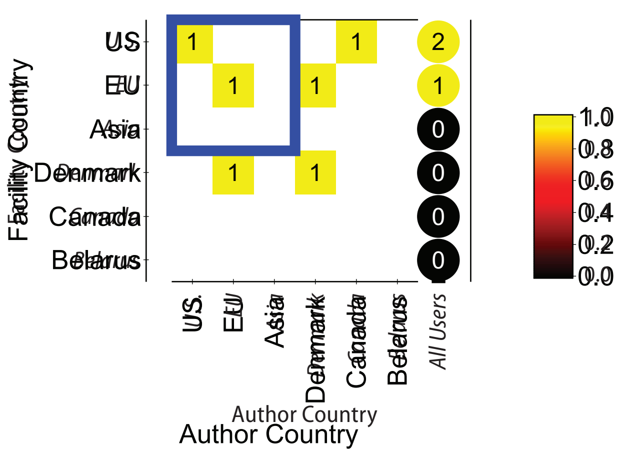


Figure A1.D



Matrix of top 1% cited papers showing the home country of the authors and the location of any facilities used. See text on page 55, "Phase 2 Methodology," for more details.

Note: Raw data are shown as markers. Solid lines have been smoothed to serve as guides to the eye.

Figure A2.A

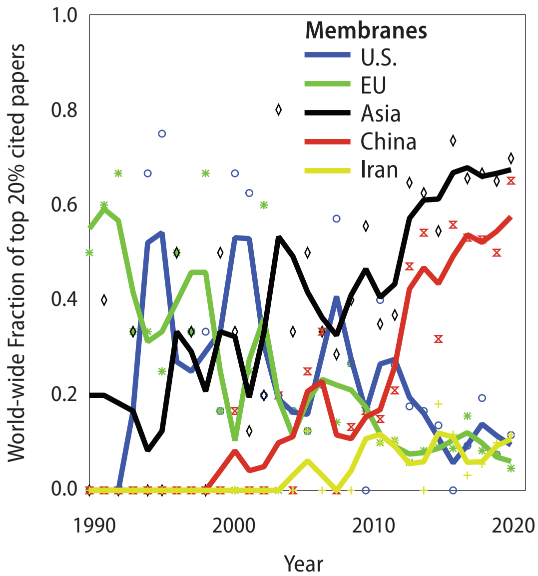


Figure A2.B

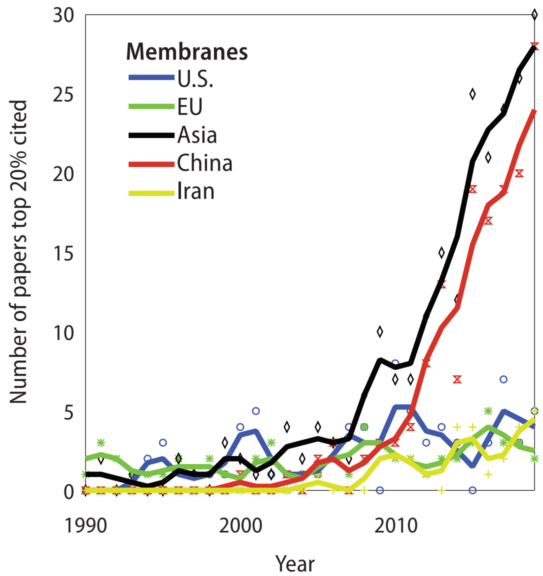
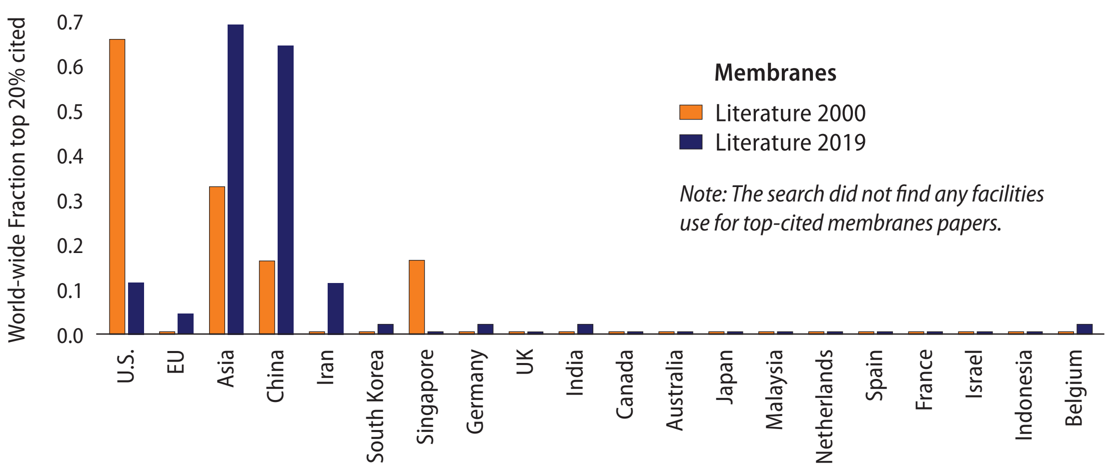


Figure A2.C



ENERGY STORAGE RESULTS

Note: Raw data are shown as markers. Solid lines have been smoothed to serve as guides to the eye.

Figure A3.A

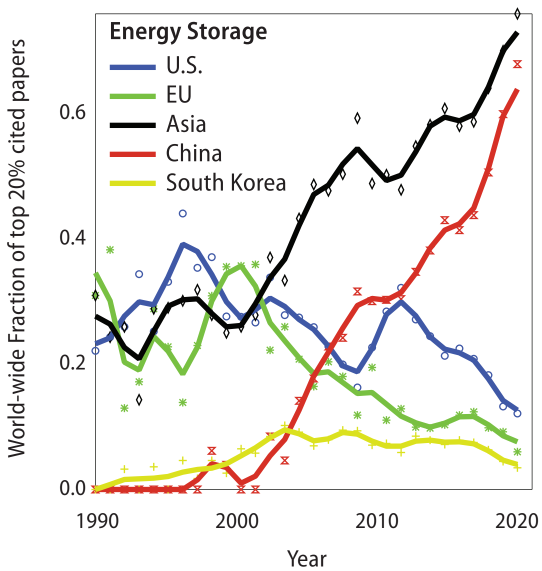


Figure A3.B

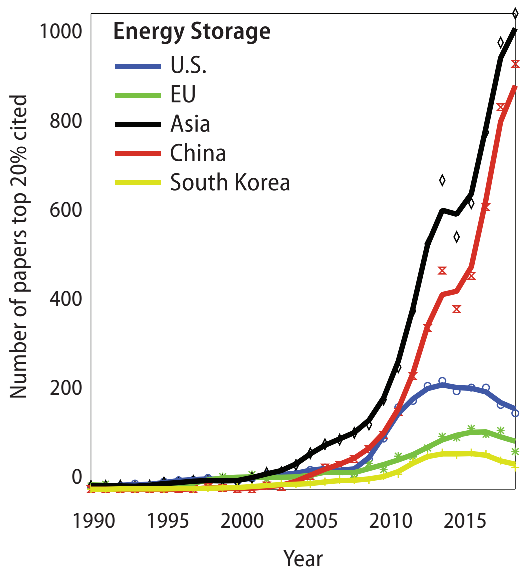
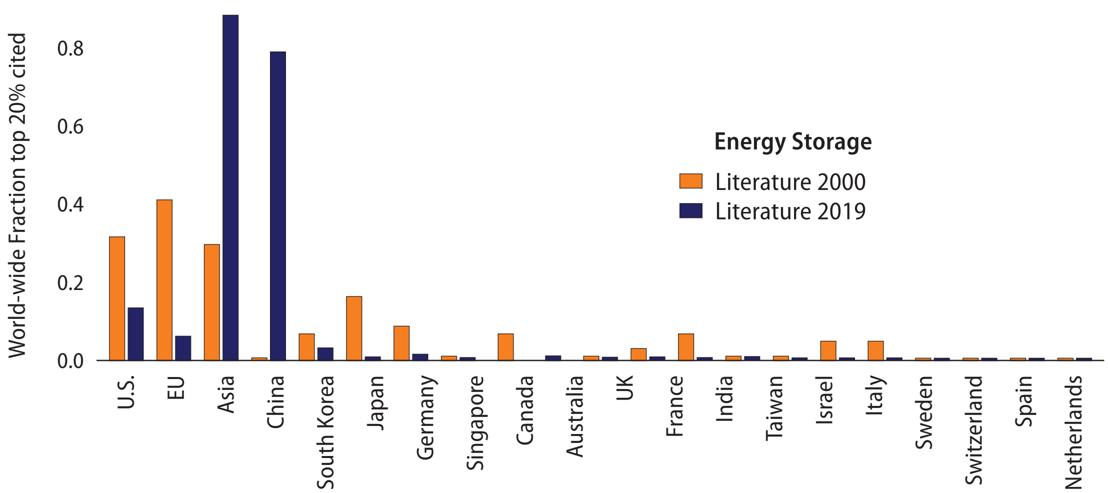
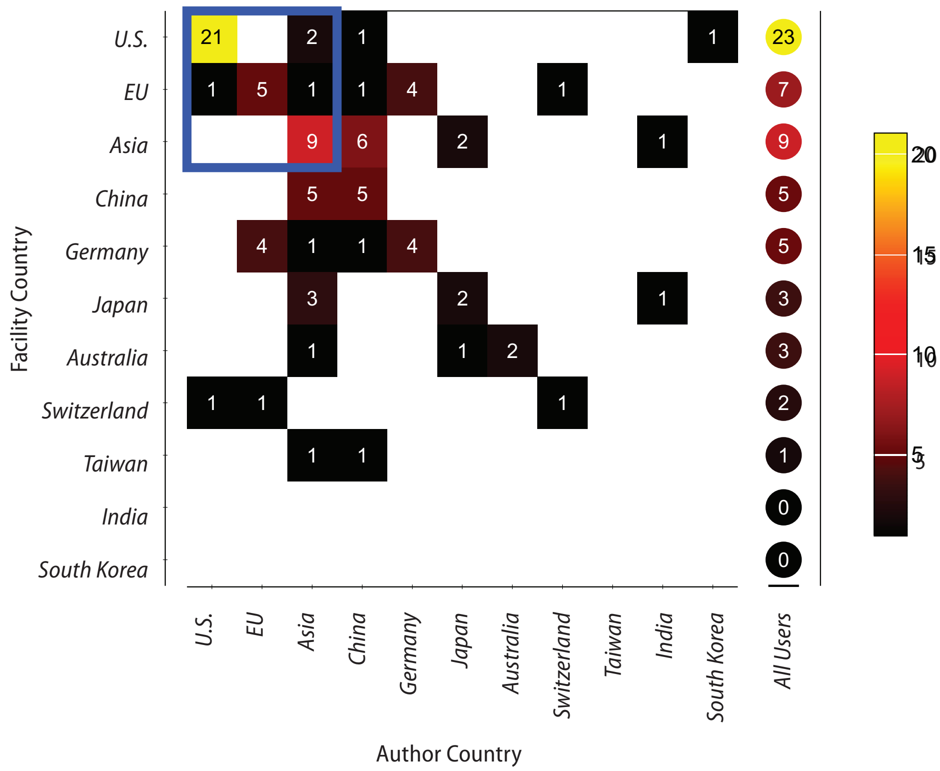


Figure A3.C



Note: Raw data are shown as markers. Solid lines have been smoothed to serve as guides to the eye.

Figure A3.D



Matrix of top 1% cited papers showing the home country of the authors and the location of any facilities used. See text on page 55, "Phase 2 Methodology," for more details.

QUANTUM MATERIALS RESULTS

Note: Raw data are shown as markers. Solid lines have been smoothed to serve as guides to the eye.

Figure A4.A

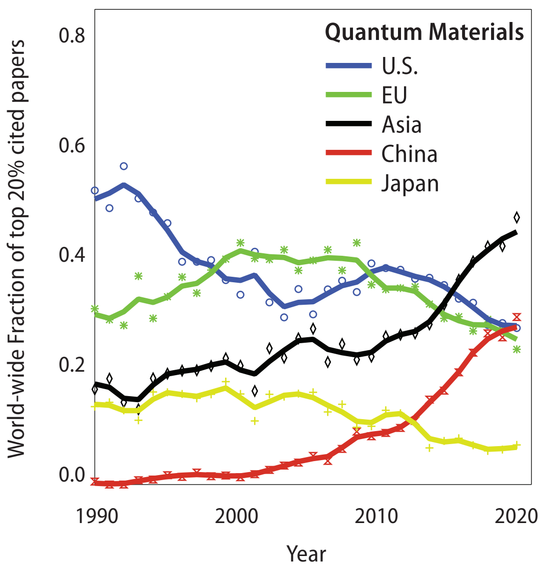


Figure A4.B

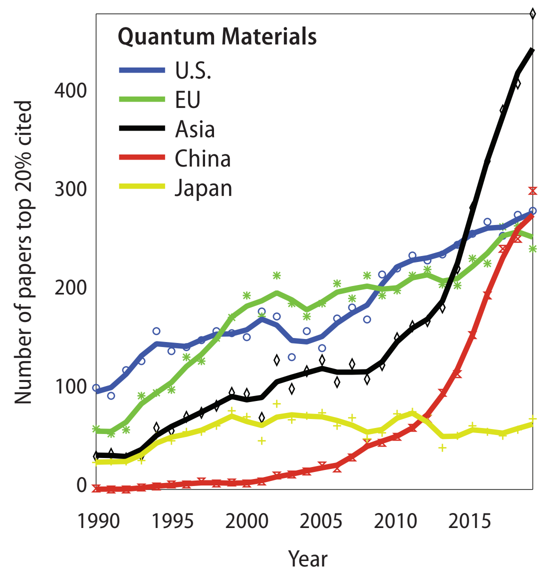


Figure A4.C

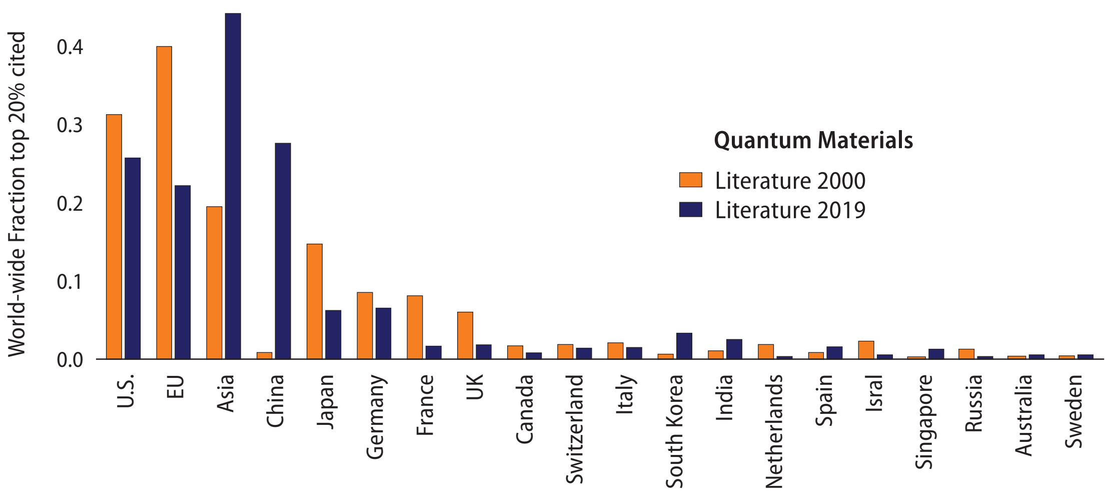
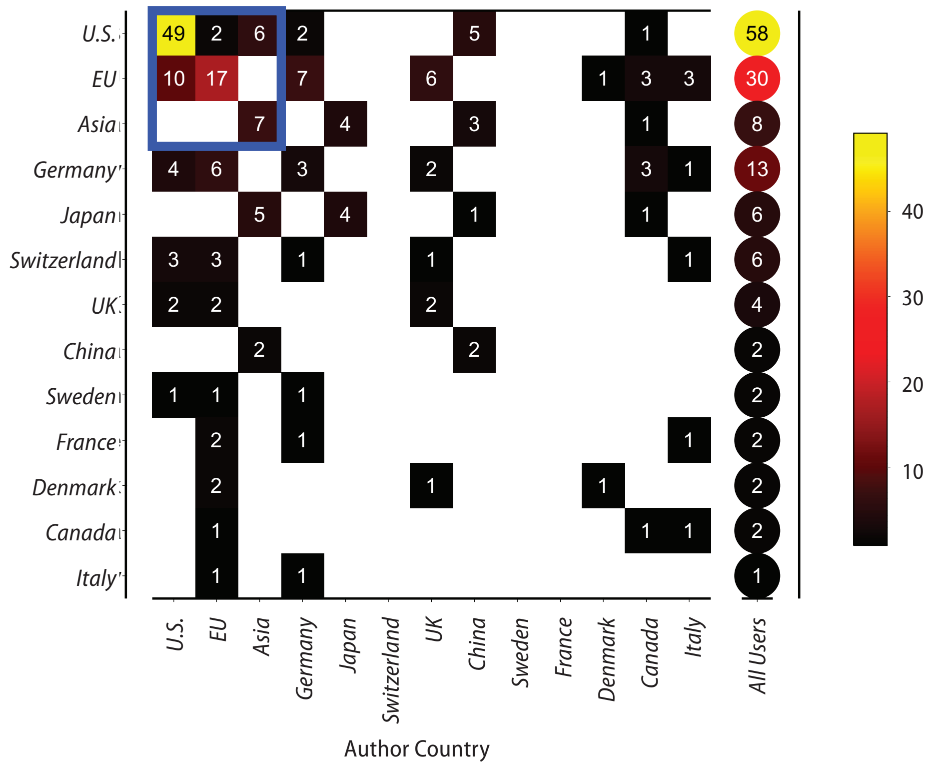


Figure A4.D



Matrix of top 1% cited papers showing the home country of the authors and the location of any facilities used. See text on page 55, "Phase 2 Methodology," for more details.

ELECTROCATALYSIS AND POLYMER UPCYCLING RESULTS

Note: Raw data are shown as markers. Solid lines have been smoothed to serve as guides to the eye.

Figure A5.A

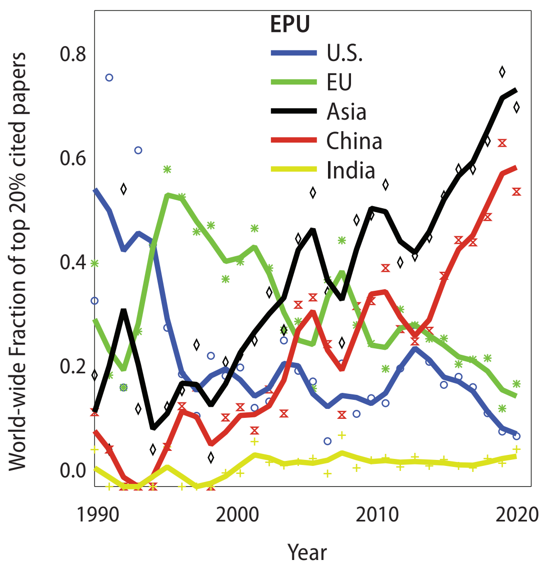


Figure A5.B

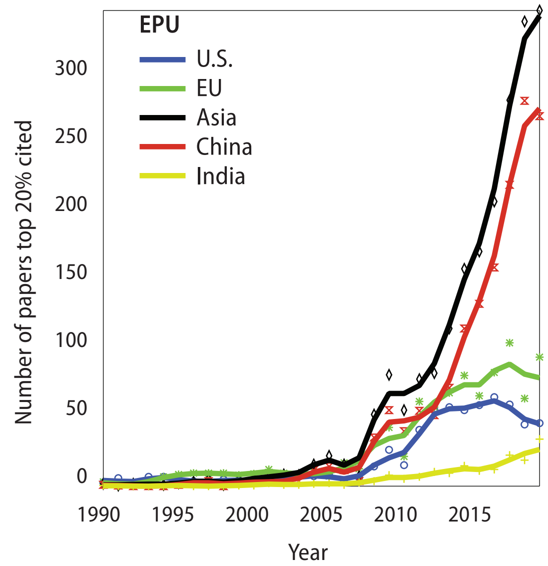


Figure A5.C

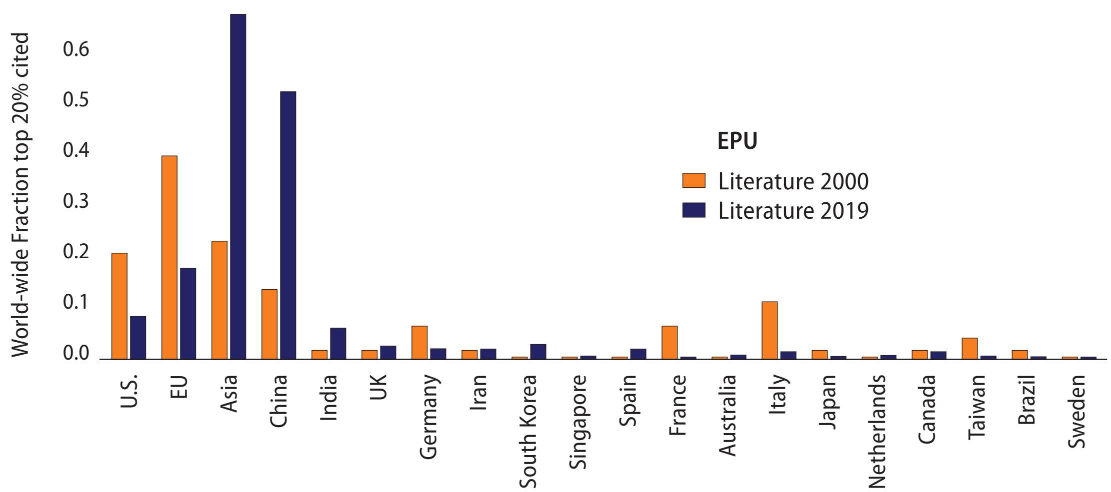
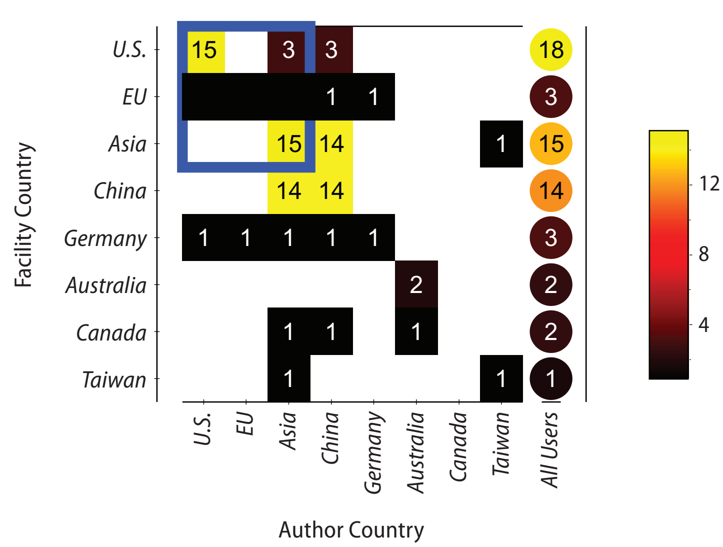
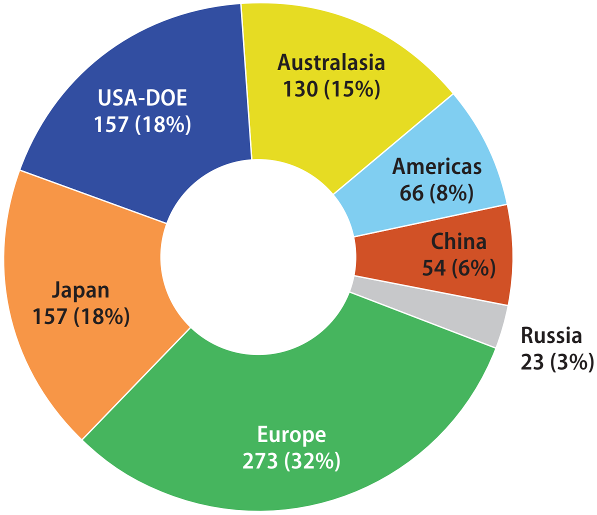


Figure A5.D

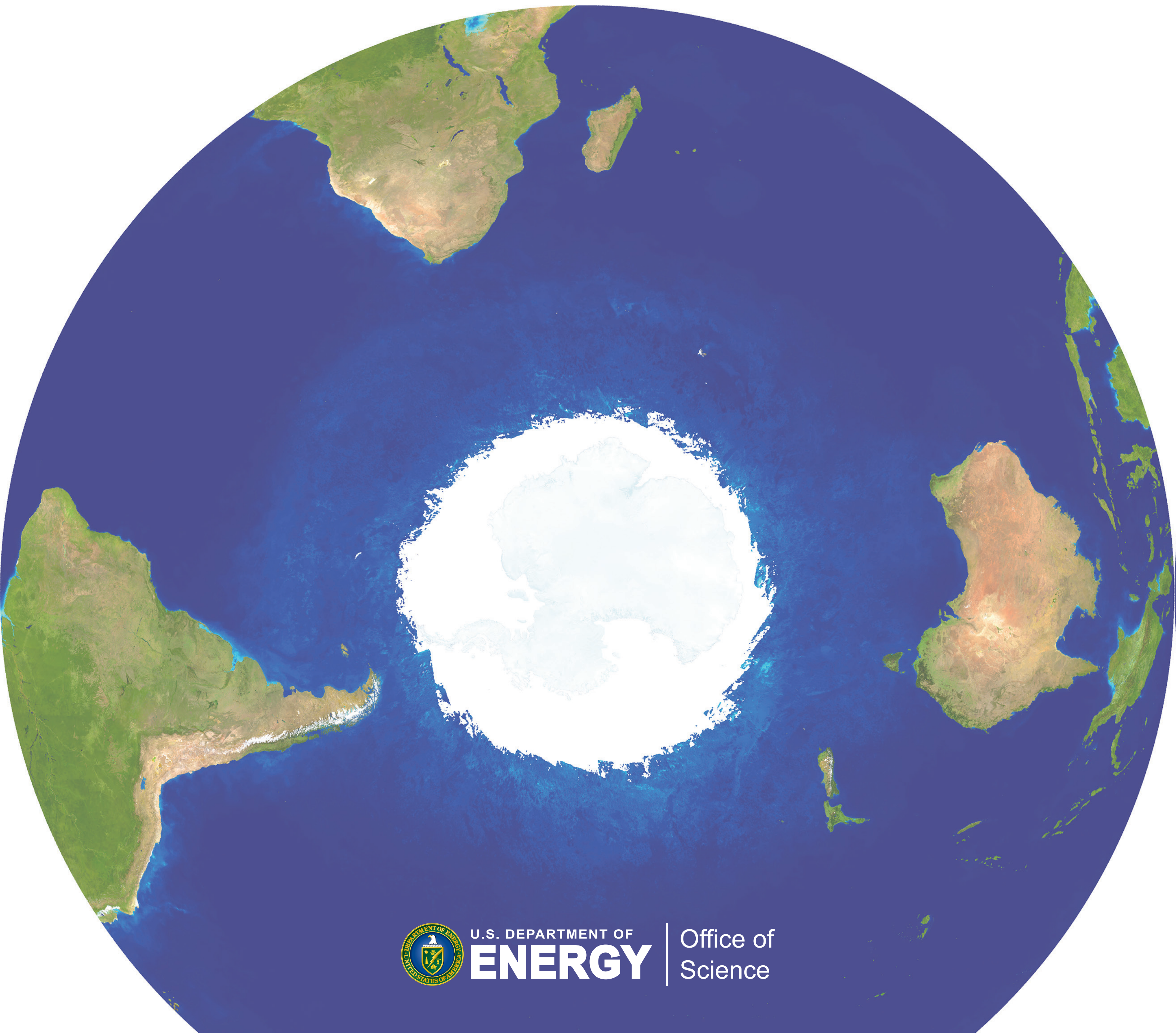


Matrix of top 1% cited papers showing the home country of the authors and the location of any facilities used. See text on page 55, "Phase 2 Methodology," for more details.

Figure A6. Detailed Breakdown as of 2021



The report is available on-line at: https://science.osti.gov/bes/Community-Resources/Reports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ENERGY
Office of
Science