# NATIONAL LABORATORIES: WORLD-LEADING INNOVATION IN SCIENCE

A Hearing of the

**COMMITTEE ON SCIENCE, SPACE, AND TECHNOLOGY**
**UNITED STATES HOUSE OF REPRESENTATIVES**

Testimony of

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## INTRODUCTION

Chairman Smith, Ranking Member Johnson, and distinguished Members of the Committee, thank you for holding this hearing and for the Committee's support for science. My colleagues at Berkeley Lab and I are particularly grateful for the legislation moved by the Committee authorizing critical parts of the Office of Science and its network of national user facilities. These bills are very important to the future of the national laboratory system. At Berkeley Lab we are particularly grateful for Congressman Steve Knight and his authorship of H.R. 4376 which authorizes the upgrade of the Advanced Light Source, one of our signature national user facilities. Thank you.

My name is Mary Maxon and I am the Associate Laboratory Director for Biosciences at Lawrence Berkeley National Laboratory, a DOE Office of Science laboratory managed by the University of California. It is my honor and my pleasure to participate in this hearing and to aid the Committee's examination of the great contributions made by the Department of Energy's national laboratories to the nation's scientific and technological innovation. Thank you for inviting me to testify.

I would also like to express my thanks and the thanks of Director Witherell and the entire staff of Lawrence Berkeley National Laboratory to Secretary Perry, Undersecretary Dabbar, Office of Science Deputy Director Steve Binkley, the Associate Directors of the Office of Science and the scores of program managers for their consistent support for what we do. Additionally, I'd like to recognize and express our appreciation for the partnership we have with the DOE Berkeley Site Office and its Director Paul Golan.

The positive engagement with the national laboratories at the highest levels of the Department has been extremely helpful and very productive. The Committee should know this, and Departmental leadership should be appropriately recognized for their strong support for the mission and well-being of the labs.

In a specific example at Berkeley Lab, we are grateful for the partnership with the Berkeley Site Office and with headquarters in the rewriting of the management contract with the University of California under the auspices of the Revolutionary Working Group contract reform successfully undertaken first at SLAC. The initiative is attempting to build upon the work and recommendations of the CRENEL report and other studies, as well as on legislation promulgated by this Committee, such as H.R. 589 that addresses the labs' ability to be a better partner for industry. The process is moving forward and we are confident that the end result will help Berkeley Lab fulfill its mission for the Department and the nation more efficiently.

My testimony will attempt to do four things.

**First,** describe Berkeley Lab and its unique role in the nation's system of national laboratories.

**Second**, describe how the national laboratories are the ultimate integrators of science and technology development for the national good. They have a unique role in the national research enterprise, one that relies on close partnerships both with industry and with academic laboratories.

**Third**, discuss why moving science and technology from the lab bench, or national user facility, to commercial viability and society is not simply a bucket brigade from research to development to deployment. Moving an innovation quickly to commercial deployment requires regular interaction between early-stage researchers, late-stage developers, and the companies that know how to introduce products into the marketplace.

And, **fourth,** explain why the national labs must not be taken for granted but nourished and supported. Countries in Europe and Asia have realized that the national laboratory system has provided a competitive advantage to the United States, and they are working quickly to reproduce it.

The investments must be made today and continually to: support cutting edge, world leading scientific user facilities; ensure the labs have secure, safe and modern infrastructure; and enhance the workforce pipeline to guarantee the recruitment and retention of diverse and world leading scientific and operations staff.

## BERKELEY LAB

Berkeley Lab was founded in 1931 by Ernest Orlando Lawrence, a UC Berkeley physicist who won the 1939 Nobel Prize in physics for his invention of the cyclotron. A circular particle accelerator, the cyclotron is the original ancestor of today's great accelerators and light sources and opened the door to high-energy physics and expedited new discoveries in diverse fields from materials and chemical sciences to biosciences and health care. Lawrence and his colleagues discovered that scientific research is best done through teams of individuals with different fields of expertise, working together. This teamwork concept is a Berkeley Lab legacy that shaped the

Manhattan Project and continues today and is reflected throughout the national laboratory complex. Berkeley Lab has moved from being a fundamental physics laboratory to one with world leading expertise and capabilities across core Office of Science mission needs and DOE applied energy research and development objectives.

With five national scientific user facilities that are utilized by around 11,000 researchers annually, Berkeley Lab is a key part of the nation's scientific and innovation infrastructure. From the world's most advanced electron microscope at the Molecular Foundry that can pinpoint how individual atoms are arranged in a material, to the world's most scientifically productive supercomputer at the National Energy Research Scientific Computing Center with its 7,000 users, researchers are attracted to Berkeley Lab, as they are to other DOE national laboratories, because of the unique capabilities and expertise they find at Berkeley Lab.

**NATIONAL LABS AS INTEGRATORS**

The Members and staff of this committee recognize well that American innovation is underpinned by a complex ecosystem consisting of people, ideas and tools that is envied by and unmatched in the world. This system grew out of a post-World War II commitment made by the federal government to support scientific research conducted at U.S. universities and national laboratories.

In today's highly competitive global environment, the U.S. innovation ecosystem is one of our nation's most precious assets. The federal government has a fundamental responsibility to keep this ecosystem healthy, because it gives the nation a powerful competitive edge, providing solutions to major national challenges and fueling economic growth. At the same time, universities and laboratories have a fundamental responsibility to be sensible stewards of taxpayer funds, conduct first-rate research on key scientific and technological problems with intellectual rigor and efficient use of resources, and strive to transfer the results of this research to industry and to markets for the benefit of society as a whole.

As many of you already know and as others will learn today, the national labs play a central role in the nation's innovation ecosystem. They are uniquely and, in some cases, singularly equipped to tackle grand challenges and opportunities because they integrate world class scientific user facilities, science and engineering experts, whole communities of scientific disciplines and researchers, and industrial needs and knowhow at a scale and breadth impossible by other institutions – in the U.S. or around the world.

Government leaders from around the world visit our national labs to understand how they are managed and organized. Some of these nations are investing heavily in an attempt to reproduce the laboratory system that we often take for granted.

Thousands of academic and industrial scientists from every state in the union, close to 1,000 from the State of Texas alone, leverage the national laboratories' facilities and scientific expertise to advance their own research. In total, over 33,000 researchers use DOE Office of Science national scientific user facilities to conduct cutting edge research. Democratic and merit based, these facilities are available to researchers with the best scientific ideas, as determined by external review committees who rank the value of the proposed research based on the quality of the science, the appropriateness to the facility, and the potential contribution to scientific knowledge. These facilities include world class supercomputers, large x-ray light sources, neutron sources and other unique instruments.

And, instead of the federal government replicating these large scale, unique facilities for each of the science agencies that require their capabilities, at a cost of billions of dollars, access to DOE scientific user facilities is agnostic to the source of funding and open to all comers - this is a tremendous asset for other federal agencies such as NSF, NASA, USDA, NIH, DOD, and NIST and for industry. Around 15,000 U.S. users of DOE's facilities have no DOE funding for their research project, a number that grows significantly if you add in researchers who are funded by DOE, other agencies, industry, foundations, and private institutions. This leveraging of DOE facilities across the entire spectrum of the nation's innovation ecosystem provides a great return on the federal investment in U.S. science infrastructure.

Additionally, the national laboratories bring together large teams of researchers to capture opportunities and address challenges at scale - much in the same way that Ernest Lawrence did in the first half of the 20th Century. It made sense then and makes a lot of sense today. National laboratories have the flexibility and the breadth to respond to national mission needs, utilizing the suite of national user facilities across the DOE complex, marshalling the research expertise of their scientists, and partnering with universities and industry. With national goals and objectives in mind, national laboratories, through the support of the Office of Science and other DOE programs, provide a longer term outlook on success. An outlook and an approach that can focus basic science capabilities on use-inspired objectives and address the challenges and opportunities from more of a turnkey perspective - taking the science from the bench, to the user facility, to collaboration with industry and finally to the marketplace.

The journey of science and technology to the marketplace and to the benefit of society does not follow a straight line. Nor is it a case of simply tossing technology over a transom to industry, hoping that its value will be recognized and that industry and investors will flock to it.  As you know, it is a much more complicated and nuanced challenge. In other words, there are no bright lines between fundamental science, applied research and development, and commercialization.

The national laboratories, in large part serendipitously, have become ideal environments in which to shepherd discoveries to the point of commercial viability - the point at which industry and investors determine that the technology is de-risked enough to attract adequate venture capital or other forms of financing. Berkeley Lab and labs throughout the complex are experimenting with new ways to engage industry and speed the delivery of novel solutions to the marketplace.  In addition to traditional technology transfer activities, such as licensing deals, royalty agreements, and spin-offs, Berkeley Lab has created new activities and have grown other, less traditional, forms of industry engagement.

One good example is Cyclotron Road.  A first of its kind program, which has now been replicated at other national laboratories, Cyclotron Road aims to bridge the “valley of death” and bring “hard” tech innovations to commercial viability by spinning into the Lab (not spinning off) small startups with big ideas.  Cyclotron Road innovators are embedded in the heart of one of the world's most formidable research and innovation ecosystems. With unencumbered access to collaborations with scientists and faculty at Berkeley Lab and UC Berkeley, its innovators are able to work hand-in-hand with world-leading facilities and experts across nearly all fields of science and engineering.

Since its founding in 2015 more than $45 million in additional early-stage funding has been generated by Cyclotron Road innovators on the basis of solid science and well prototyped technology. And because the small start-up companies that “spin in” to the national lab are largely comprised of early career researchers, the Cyclotron Road effort may well be on its way to training the next generation of industry leaders through a novel partnership paradigm where national lab assets and experienced mentors can greatly accelerate the success of small companies.  From materials and manufacturing, to electric power and storage, transportation, and electronics and computing, Cyclotron Road’s innovators are developing technologies across a broad range of fields and industries with the potential to transform the world.

Berkeley Lab, as other national laboratories do, continues to attract and work with industry through the national user facilities and large research programs such as the Joint Bioenergy Institute and the Joint Center for Artificial Photosynthesis. Increasingly, industry reps are serving key roles on lab and research advisory boards and review committees.

**OPPORTUNITIES**

By now, most of you and much of Washington understand that some of our nation's scientific infrastructure is old - a lot of it, in fact - including at our national laboratories. Even so, our entrepreneurial spirit, our ecosystem of innovation as described above, and our culture of creativity and discovery continue to provide us with inherent advantages.

Times are changing however. Learning from our success, other countries are building more technologically advanced light sources, bigger laser research facilities, more powerful supercomputers, etc. The time is now for the United States to invest and ensure that our advantages don't disintegrate and leave us behind in the delivery of key scientific resources and capabilities to American researchers at the labs, in academia, and within industry.

**World Leading Scientific Facilities**

That is why this Committee's action on user facilities and the Department's initiative to upgrade its national user facilities are so very important. Young, passionate scientists, especially the best of the best, will have to go where they can conduct the most cutting edge and transformational research. As a nation, we must ensure that the place to do that is here, at our national laboratories, at our universities, and within our industries. The President's budget contains good news on this front, especially for the Office of Science Basic Energy Sciences program and its light sources. Berkeley Lab is particularly pleased with the FY19 budget's proposed funding for upgrading the Advanced Light Source. After its upgrade, the ALS will be the premier light source in the world for the delivery of soft x-ray light and should retain this title for years - attracting the best of the best from the U.S. and from around the world.

We are also excited about the Department's exascale computing initiative and Berkeley Lab's role in bringing it to productive fruition. Congressional leaders on this Committee, like Congressman Hultgren, Congresswoman Lofgren and others, have made the nation's high performance computing capabilities a key focus of their policy goals and early on led the fight to advance U.S. supercomputing. As we embark on the path to exascale computing, Berkeley Lab's NERSC, the workhorse computing facility for scientific output for the Office of Science research programs, looks forward to delivering exascale capabilities to the broader scientific community.

Additionally, the Congress and the Department have demonstrated their support for upgrading ESnet - DOE's advanced scientific network. ESnet currently moves ~730 petabytes of data per year. With exascale capable computers coming online the size of yearly data is expected to increase to ~7 exabytes in 2021. For context, remember that 1 exabyte is a unit of information equal to one quintillion (10 to the 18th) bytes, or one billion gigabytes. ESnet's upgrade is critical to the success of the Department's exascale program.

**<u>Plant and Facilities Infrastructure Renewal</u>**

An issue that you may not know about is the state of our national laboratories' basic plant infrastructure - the electrical and water systems, the condition of the building stock, roads, etc. Because the labs are old - several buildings at Berkeley Lab that are still in use today were built in the 1940s - and because the pace of maintenance, repairs and replacements have not kept up with the need, there is now a large and expensive backlog of deferred actions. At Berkeley Lab, the estimated cost of deferred maintenance is significant. Although much of it is non-critical, some of it is. This scenario is repeated across the entire laboratory complex.

Fortunately, over the past several years, DOE's Office of Science Science Laboratories Infrastructure office has engaged in a proactive and prioritized strategy to first deal with the most urgent issues and to work its way down the list across the entire laboratory complex. All the Office of Science laboratories have benefited from this strategy. At Berkeley Lab, we have been able to tackle critical infrastructure needs and have replaced subpar and unsafe structures with new facilities. Currently, Science Laboratories Infrastructure is constructing the Integrative Genomics Building at Berkeley Lab. This state of the art building will house the Joint Genome Institute, currently located 20 miles away in Walnut Creek, California, and KBase. Both programs are described later.

Even though progress is being made, it's a hard job, deciding how much funding to divert from science for more mundane, if critical, basic infrastructure projects. Ultimately, however, this is a false choice - a commitment must be made to do both. Failing basic infrastructure makes the science superfluous. I urge the Committee to explore the infrastructure issue and to work closely with the Department and the White House and with the appropriations committee of jurisdiction to find solutions to this long term challenge.

**Ensuring a Diverse and Talented Workforce**

Another critical part, the most important part, of the nation's scientific infrastructure are the men and women who conduct the science as well as those who provide the much needed administrative, financial, technical, and health and safety support. Although the narrative of the brilliant solo scientist persists in today's culture, in fact most scientific research is conducted by teams of people rather than single investigators. Scientific discovery is fueled by creativity and perseverance, and progress is often made when diverse perspectives allow problems to be seen from a variety of different angles.

Successful scientific work environments are those where promising new ideas are fostered and researchers are encouraged to push beyond conventional schools of thought. At national labs, researchers from a broad range of scientific disciplines who have been trained at universities around the world come together to solve national-scale challenges, and many of those challenges sit at the intersections of scientific fields where expertise in single disciplines is insufficient to address them. Supporting these challenging research efforts are dedicated operations staff, without whom scientific progress would be impossible.

Cultivating talent and promoting inclusion is central to the creation of a successful work environment driven by a diversity of thought partners working toward shared objectives. Among the national labs, Berkeley Lab was the first to publish its workforce diversity demographics. From the undergraduate population through senior lab leadership, Berkeley Lab tracks and posts its numbers of women, under-represented minorities, other people of color, two or more races/ethnicities, and whites.

Berkeley Lab believes that with greater diversity in our leadership and throughout the lab, more family-friendly policies, and training in implicit bias for search committees, we have made a strong start. But it is only the beginning of a process that requires continual improvement. We are committed to long-term efforts to ensure that diversity, equity, and inclusion become hallmarks of the Berkeley Lab culture. Though this will require steady attention and effort, we know that our success as a national lab depends upon our ability to create a community that brings together people with diverse backgrounds, points of view, and approaches to problem-solving, and who are committed to bringing science solutions to the world.

**CONCLUSION**

Thank you, again, for the opportunity to testify at this important hearing. In summary, I applaud the work of the Committee to address the following issues and encourage you to continue to work together, with the Administration, and with other key committees to continually make progress on:

- Ensuring U.S. international leadership in the delivery of state of the art national scientific user facilities with cutting edge research capabilities;
- Explore ways to address the much needed renewal of the national laboratories' aging plant and facilities infrastructure;
- Examining and creatively approaching new ideas to increase the diversity of our national laboratory workforce in ways that attract the best of the best.

Finally, below are examples of science at Berkeley Lab and among our partners and collaborators that illustrate how national labs succeed through integration of resources and capabilities.

I am happy to answer any questions and Berkeley Lab is always pleased to assist the Committee in its work on issues of national importance.

## EXAMPLES OF SCIENTIFIC AND TECHNOLOGY INTEGRATION AND INDUSTRY ENGAGEMENT

### 1. BIOSCIENCES

While Berkeley Lab may be best known for its physical, chemical, and material sciences, the biological sciences have been part of its DNA almost from the beginning when Lawrence recruited top-flight scientists to UC Berkeley in the 1930s.

Lawrence's younger brother John, a physicist and physician, is considered the father of nuclear medicine. At Berkeley Lab, John studied the biological effects of the byproducts of the atom smashers Ernest built, and carried out the first successful treatment of human disease with radioisotopes. Today nuclear medicine still plays a central role in the diagnosis and treatment of cancer and other human diseases, and today's health-related scientists at Berkeley Lab are building on these foundations in their research efforts to better understand cancer, DNA repair, genome structure and function, and neurodegenerative diseases.

Biochemist Melvin Calvin used radioactive carbon-14 from a Berkeley Lab cyclotron to map the route that carbon travels through a plant during photosynthesis — research that led to discovery of the "Calvin cycle" and the Nobel Prize in Chemistry in 1961. Today's physical bioscientists and engineers at Berkeley Lab are building on advances in the physical sciences and modern biology, including those of Calvin, to examine, characterize, and mimic biological molecules and molecular functions to create unique biological structures that can then be used to solve some of the 21st century's most difficult fundamental research problems.

Berkeley Lab conducted path-breaking research on medical imaging, including early development of computed tomography (CT) scans and positron-emission tomography, (PET) scans. Cancer studies broadened to include tracking the behavior of healthy and malignant cells in culture and animals, pioneering the development of 3-D human tissue models, defining cancers as diseases of tissue microenvironments, and identifying many of the impacts of radiation on cells and organisms. Studies of heart disease and Alzheimer's disease helped to characterize the role of oxygen radicals in aging and disease. Bioscience research at Berkeley Lab deepened our understanding of what was becoming known as "systems biology."

The extensive work in biological sciences and pioneering studies on mapping and sequencing the genome of the model organism *Drosophila melanogaster* led to selection of Berkeley Lab as one of five centers for the Human Genome Project, the massive national effort to map and sequence the entire complement of human DNA. Berkeley Lab's Human Genome Center, which was consolidated into the Department of Energy Joint Genome Institute (the DOE JGI) in Walnut Creek, was responsible for sequencing a significant portion of the human genome. Since that time, the DOE JGI has undertaken a considerable effort to determine the genome sequences of thousands of plants and microorganisms with the aim of using this genomic information to develop solutions to national-scale energy and environment challenges.

Aided by faster computers and more advanced algorithms, studies of gene regulation intensified. Berkeley Lab played a major role in the Model Organism Encyclopedia of DNA Elements Project, which resulted in greatly improved genome annotations and scientific understanding of non-protein coding RNAs, chromatin "landscapes," and genome functions. Rapid sequencing renewed interest in proteins, including how they are structured and how they work. X-ray crystallography at the Advanced Light Source, plus a range of powerful microscopic techniques, revealed structures of important proteins at the highest resolutions ever.

The focus on genetics and molecular biology developed naturally toward the discipline now called synthetic biology, which holds the promise of reducing dramatically the costs and time required to design, build, and characterize biological systems. These innovations have led to focused applications and the creation of a number of spin off companies.

The United States has the potential to produce over 1 billion tons of non-food, non-feed biomass that can be mobilized to expand the bioeconomy. In 2012, the National Bioeconomy Blueprint highlighted the opportunities in energy and manufacturing resulting from this strategic resource. Recent assessments have concluded that these opportunities could expand the bioeconomy, adding $259 billion and 1.1 million jobs to the US economy by 2030. Berkeley Lab embarked on an intensive effort to use the tools of genetics, supercomputers, and microbiology to develop biofuels and new sources of sustainable energy. The Joint BioEnergy Institute is one of three national centers created by the DOE in 2007, and expanded to four in 2018, to advance the development of biofuels and biomass derived products.

Building on a legacy of advanced research in biosciences, Berkeley Lab has the infrastructure and expertise to bring biological solutions to the energy, health, and environmental challenges of our time as well as provide the foundational underpinnings for a strong biological manufacturing industry.

In addition to our focus on using science to bring solutions to the world, our strategy also embraces a Berkeley Lab commitment to transferring our knowledge to our surrounding communities. We will continue to combine our research efforts with efforts to reach out to our neighbors. Through workshops, internships, and educational programs at local schools, colleges, and universities, we will promote understanding of science and encourage young people of diverse backgrounds to make a career in biosciences part of their own strategic plans.

Today, I'd like to share some examples of how Berkeley Lab's Biosciences programs address national-scale scientific challenges.

**Genomic Sciences**

Genome sequencing has evolved from a highly-specialized technology requiring rooms of equipment to one that will soon be democratized through the use of small, portable sequencers barely larger than a thumb drive. At the same time as the speed and availability of sequencing is increasing dramatically, ever more complicated organisms and now communities of microbes are being sequenced. Indeed, the diversity and scale of data generation is growing significantly across the spectrum of biological research, including genome data, advanced imaging analyses, diverse measurements of biomolecular structure and function, spatial and temporal structuring of biological system population genetics, biologically influenced environmental processes, metabolic modeling, and an expanding array of fermentation processes for fuels and chemicals. Biological data generation is increasing at a rate that outpaces Moore's law, meaning that we cannot rely on hardware alone to tackle these data challenges. Scientists and engineers, drawn from across the national lab complex, will be needed to develop new algorithms, standards, and tools that ensure access of biological scientists to state-of-the-art high performance computing. This will be particularly important in the exascale environment in which hardware and software are likely to be co-designed for specific applications.

Recognizing that data collection and standardization will be crucial for unlocking new insight into microbial community functions and importance, Berkeley Lab is leading efforts, with university partners, to establish the National Microbiome Data Collaborative. The collaborative will be a hub for microbiome data and related analysis tools. In addition to this effort, Berkeley Lab is home to the DOE Joint Genome Institute and the DOE Systems Biology Knowledgebase. As I mentioned earlier, the Joint Genome Institute provides advanced genome sciences technologies for scientists studying organisms important to DOE's energy and environment missions. The Systems Biology Knowledgebase is a platform for data and tools designed to accelerate research about microorganisms, plants, and their communities in an environmental context with an emphasis on DOE goals. It makes these data and tools accessible to scientists in a user friendly format, allowing them to gain tremendous insight into the workings of organisms without need expertise in data and computing sciences. The Joint Genome Institute and the Systems Biology Knowledgebase are integrating their data and platforms, allowing users around the world unparalleled access to their expertise in genome sciences, data analysis, metabolic modeling, and computational methods for application to challenging questions in energy and environment.

**Advanced Biofuels and Bioproducts**

Central to the mission of the DOE national labs is developing the fundamental science and technologies that will ensure that the U.S. can meet its energy needs. Biology can play a significant role in this space to create the bio-based fuels, chemicals, and products that utilize our strategic biomass resources. Converting the billion tons of potentially available non-food, non-feed biomass into useful materials requires fundamental and use-inspired research and development to develop efficient biological conversion processes. These approaches draw inspiration from nature by manipulating the natural processes within organisms and from the ways that humans have used microorganisms and fermentation to create food and beverages. The Joint BioEnergy Institute (JBEI), established in 2007 and recently renewed in 2017, takes an integrated approach to developing new bio-based fuels and chemicals. JBEI is based on the concept of integration - bringing together under one roof the expertise, knowhow and unique resources of five national laboratories and six universities from around the nation, and with the collaboration and integration of industry researchers, all working side by side with shared objectives.

Researchers at JBEI are probing the biological mechanisms behind biomass structure and resilience in order to develop better bioenergy crops that can be more readily deconstructed to useful molecular building blocks and that can withstand environmental stressors. Other members of the JBEI team are developing new bioenergy crop deconstruction approaches that are efficient and minimize contamination. JBEI scientists are also engineering microorganisms to convert the biomass building blocks from deconstruction processes to gasoline, jet and diesel fuels, and useful bioproducts that can reduce the overall cost of production. All of these efforts are underpinned by technology development that strives to increase the throughput and efficiency of production while minimizing costs, time, and energy intensity. Since its inception, JBEI has demonstrated an impressive track record of success in driving solutions to the marketplace. The numbers tell a great story: 713 publications; 26,600,000 citations; 89 IP licenses; 174 patent applications; 35 patents issued; and 6 startup companies.

Another multidisciplinary team science approach to solving national-scale biological challenges and driving the national bioeconomy is the Agile BioFoundry. The Agile BioFoundry was established, in response to industry need, as a consortium of eight national labs (Argonne, Berkeley, Idaho, Los Alamos, NREL, Oak Ridge, Pacific Northwest, Sandia) in 2016 by DOE's Office of Energy Efficiency and Renewable Energy. It aims to unite the unique and differentiated capabilities of the national labs to develop an integrated biological engineering platform that can reduce the time and cost of producing biofuels and bioproducts. The core of the Agile BioFoundry platform is an integrated Design-Build-Test-Learn cycle meant to speed the development of new production organisms by applying machine learning and statistical methods to designing biological routes to products while incorporating techno-economic analyses, life cycle assessments, and measurement at industry scales. Many of the technologies that are being implemented in the Agile BioFoundry were initially developed at the Bioenergy Research Centers, and many more are being jointly developed by the eight national lab team; the Agile BioFoundry is integrating those technologies and de-risking them for eventual implementation by industry.

The Agile BioFoundry was established in response to a number of industry listening days where industrial biotechnology company representatives articulated research needs that were beyond their capacity to address. The first listening day in 2013 was held in Washington, D.C. to bring together thought leaders from industry with Federal funding agencies. These discussions highlighted the "valleys of death" between the published work performed at universities and at the national labs funded by the U.S. government and the what is considered "ready" for commercialization by industry. In the industrial biotechnology industry, these valleys include computer-assisted design tools for designing organisms that can produce products of interest to industry, optimized organisms that can reliably produce these products at scale, and cutting-edge analytical technologies to assess production efficiently. Two additional listening days were held, one in Berkeley, CA and one in Washington, D.C., to engage industry members in the planning of the Agile BioFoundry. These listening days served two purposes- first, to identify the core pre-competitive technologies that the Agile BioFoundry could de-risk for industry; second, to ensure that the Agile BioFoundry brings the full value of the national lab capabilities to bear on challenging biological engineering problems that industry cannot solve alone.

Many technologies developed through fundamental or use-inspired research are proof-of-principle and not yet suited for deployment in the private sector, and a need exists to more fully develop or “harden” the technologies for use in production settings. The Agile BioFoundry runs campaigns to continually improve predictive design tools and to generate publicly accessible data about organism performance and pathways for full public benefit. And in an effort to identify and address more specific challenges that would benefit industry advancement broadly, the Agile BioFoundry has embarked on seven two-year projects with small companies resulting from a recent solicitation where companies were invited to submit proposals for Agile BioFoundry consideration. Some of the chosen projects focus on the informatics tools and data analysis activities of interest to industry while others support the development of key microbial organisms that may eventually be commercialized. The Agile BioFoundry’s recent solicitation shows that there is significant demand for this type of national lab research; 19 companies applied for a total of $20M in requested funds, four times the amount of funding available through the solicitation. The Agile BioFoundry established an industry engagement team comprised of industry advisors who help to continually assess the pre-competitive challenges that the Agile BioFoundry could address for and with the industrial biotechnology industry.

**Microbiome Research and Development**

Berkeley Lab researchers and scientists across the national lab complex are at the forefront of microbiome research for energy, environment, and agriculture. Most people don’t know it, but there are more microbes in a handful of dirt than there are stars in our galaxy. And, these microbes don’t exit as solitary entities, but as actors in a well choreographed interchange of activity - activity that determines much about the health and wellbeing of their environment and ultimately of their larger biomes.

Scientific focus areas like the ENIGMA, funded by DOE’s Office of Science Biological and Environmental Research program, enable multidisciplinary research that can investigate microbiome function from the molecular level or an individual organism to the interactions of whole communities of microorganisms in field sites. ENIGMA aims to understand how environmental contamination affects these microbial communities and perhaps one day, identify methods to mitigate contamination. ENIGMA has already led to significant improvement in our understanding of how microbes interact with each other and technologies developed to probe these interactions have been shown to have broad applicability beyond this project, winning R&D100 awards.

Despite the recent explosion in microbiome research, an enormous knowledge gap remains. More research is needed to understand microbiome function, how those functions might be manipulated, and how manipulation of microbiomes can be used for application in energy, environment, and agriculture. To truly interrogate this space, collaboration across many scientific disciplines -- biology, ecology, physics, mathematics, computing -- is required, and national lab capabilities are ripe to address many of the research challenges in microbiome science. Through the manipulation of microbiomes, one can imagine bioenergy crops developed with microbiomes that promote growth and mitigate stressors so that these crops can be grown on marginal lands with minimal fertilizer and water. And one could use tailored microbiomes to remediate contaminated soils, making them amenable to agriculture, construction, or recreation. Microbiome-based fermentation could also be used to convert waste gases such as carbon dioxide and methane that pollute our environment to valuable products. These are just a few applications that could be realized as a consequence of a deeper understanding of microbiome structure and function.

The research and development needed to make progress on all these fronts will require an approach that includes biologists, ecologists, chemists, computer scientists, mathematicians, and statisticians in a coordinated manner. Beyond the scientific questions, new technologies will be needed to manipulate microbiomes and to ensure that findings in the lab are reproducible in the real world. Efforts like the National Microbiome Data Collaborative and the DOE Systems Biology Knowledgebase will be essential for ensuring that microbiome data and analyses can be shared broadly and systematically for development of new products and services. And this can’t be done alone- national labs must work with industry, who will commercialize microbiome technologies, and regulators to ensure that applications of microbiome research are safe and provide value to the American public.

## 2. HIGH PERFORMANCE COMPUTING AND ADVANCED NETWORKING

A revolution is underway - steadily and unmistakably - in many scientific domains and we have reached an inflection point. Scientists are developing new tools to access, manipulate, analyze, combine, and re-purpose complex datasets. At the same time, they are using sophisticated mathematical analyses and simulations to drive the discovery of relationships across datasets. Across many fields of observational and experimental science, data-rich discovery environments are emerging. Assembling these environments takes three ingredients: high performance computing and networking resources for data processing, transfer, storage and analysis; scalable and flexible software tools and applications; and highly skilled experts - including mathematicians, engineers, and computational and domain scientists. Each ingredient is important. When carefully integrated, they can render large-scale datasets that are tractable and useful. Effective discovery environments for extreme-scale data promise many benefits, including more insight per experiment, higher quality results, greater impacts for facilities, and increased democratization of science. New data analysis techniques will enhance, not replace, theory and experiment as techniques for inquiry.

At Berkeley Lab, our vision is the development of a “superfacility” that closely binds user facilities, experiments, and users with HPC computing and advanced networking. This Superfacility will transform science through a network of connected facilities, software, and expertise to enable new modes of discovery. This isn’t a brick and mortar facility, but a virtual one that connects assets and squeezes out more knowledge, more efficiencies, and a higher return on the federal investment.

In particular, we envision an experimental facility (such as a DOE Office of Science light source), one or more data management and processing facilities, and the network fabric and software infrastructure to bind them all together as an integrated Superfacility which provides seamless, real-time access to the capabilities of both data source and data analysis facilities as one. An end-user of an experimental facility would operate as though at a single facility, without knowledge that they are actually using multiple DOE user facilities.

As an illustration, a user might begin to conduct an experiment at a light source end station; preparing and placing their experimental sample; tuning the beamline optics and configuring the Data Acquisition (DAQ) system; run QA tests, then the actual science-driven experiment; and see the fully-processed results on their monitor alongside the beamline controls and DAQ -- never realizing that the processed results shown required transfer of data, marshalling of real-time compute resources, execution of a complex analysis chain incorporating advanced mathematics and analytics, and visual presentation of results back to the end-station. Such a user would never need to worry about multiple user accounts and permissions; never need to know about queues and compute architectures; or ever concern herself with inter-process communications or any of the other details of how the processing happens.

Berkeley Lab Computing Sciences, ESnet, NERSC, and the Computational Research Division have begun to partner with DOE experimental facilities, such as the Advanced Light Source, to automate pipelines to run on HPC systems, improve network transfer rates between facilities, create new mathematical techniques for data analysis and develop software tools to aid in the sharing and curation of data.

**Unlocking Secrets of Proteins - Never Before Seen Macromolecular Structures**

Photon science experiments at facilities such as the ALS, LCLS, and NSLS-II, enable scientists to resolve the structures of macromolecular protein complexes that were previously inaccessible, capture bond information in the elusive transition-state of a chemical reaction, and probe the extreme states of matter. These light sources come with varying numbers of instruments arranged in a tight cluster. Some of the detectors on these instruments now generate terabytes of data per sample. While beamline scientists were once able to carry data home on a flash drive, massive increases in spatial and temporal resolution has lead to increasing data set sizes and the need to look for new solutions for data analysis.

The computational challenge for light source data analyses is to reduce the time to solution from weeks to minutes with real-time interpretation of molecular structure revealed by X-ray diffraction, while dramatically increasing the experimental throughput. For example, the LCLS detector rates will increase 1000-fold by 2025. Recent work with Berkeley Lab's Computational Research Division (CRD), ESnet, NERSC, and ALS along with partnerships with SLAC's LCLS facility has informed what is perhaps a growing trend at DOE Light Sources. If sufficient bandwidth can be provided then a shared high-performance computer, coupled with fast storage, can provide beamline scientists access to large scale resources and faster time to solution. Faster data analysis in practice can mean spotting errors in sample handling or experimental setup, and numerous other issues that can bring beamline progress to a halt and slow scientific discovery.

**What to do with the Explosion in Biological Data?**

Over the past 2 decades there has been an explosion of biologic data production, and the DOE science-complex has been and will continue to be a major contributor to this data deluge. Berkeley Lab scientists envision using this vast trove of data to solve major problems in energy and environment through the creation of new models of biological function that enable prediction, control and design of biomolecules, microbes, plants, and biomes. This vision requires not just the analysis of large volumes of data, but also the integration of a variety of different kinds of data, spanning -omics, images, and sensors, across time scales from nanoseconds to years.

DOE’s leadership in high performance computing positions the national laboratories well to address this challenge, but it is important to recognize that performing biological computing on supercomputers requires significant modification to algorithms and software currently employed for this task, as well as a commitment by supercomputing facilities to understand the needs of the biology community. This will not happen without significant investment in the specific problem of high performance biologic computing and will require the collaborative effort of biologists, bioinfomaticians, applied mathematicians, and computer scientists.  Success in this endeavor will have benefits reaching well beyond DOE's mission space to the public sector including health, agriculture, and biomanufacturing industries. This is a hard problem whose benefits justify focusing the national lab complex's expertise and capabilities on it.

**Materials by Design with High Performance Computing**

Advanced materials are essential to economic and societal development, with applications in multiple industries, from clean energy, to national security, and human welfare. Historically, novel materials exploration has been slow and expensive, taking on average 18 years from concept to commercialization. Traditional empirical and 'one-at-a-time' materials testing is hence unlikely to meet our future materials innovation challenges in a timely manner. However, due to tremendous improvements in computing, coupled with software development during the last decades, real materials properties can now be calculated from quantum mechanics – *much faster than they can be measured.* A new era of computational materials prediction and design has been born.

In 2010, Berkeley Lab saw this opportunity, and by leveraging team expertise in multidisciplinary areas spanning software design, computing, and materials science, created the first open online materials database by enabling thousands of automatic calculations per week – enabling screening and predictions - for both novel solid as well as molecular species with target properties. Since then, the *Materials Project* (www.materialsproject.org) has been constantly computing the properties of all known inorganic materials and beyond, and disseminates the results freely to the public. This 'google of materials' allows students, researchers, and industrial engineers to ask informed questions that translate into 'give me all safe Li-ion battery materials that can run an electric car for 300 miles' and it will produce a long list of structures and chemical systems which have the potential to satisfy the criteria. The current release contains data for over 70,000 materials with millions of associated properties and the numbers grow daily. As a testament to its popularity, the Project has over 45,000 registered users worldwide, and thousands log into the web site every day and use the resource. Several examples of novel materials that were designed using the data and design resources span the breadth of novel waste heat recovery materials, new battery materials, new solar fuel catalysts and new sensor materials, that can enable new industries and new solutions to technological challenges.

## 3. DRIVING ENERGY SOLUTIONS TO SOCIETY

Basic science forms the foundation that our nation's technology solutions are built on. From that bedrock, the national laboratories have built strong partnerships with industry to move use-inspired technologies out of the lab and closer to commercialization. Berkeley Lab has contributed to the development of many high profile technologies that improve our lives and contribute to the American economy. One example is the class of materials known as "quantum dots" – nanoscopic semiconductor crystals that are finding a wide range of applications today, in everything from QLED TVs, to light bulbs, to biomedical imaging, and more. Berkeley Lab's decades of basic research to explore and improve the useful properties of quantum dots led to a valuable patent portfolio, licensed by U.S.-based companies to commercialize the use of quantum dots in several different fields of use. Emerging applications of quantum dots include targeted cancer therapies and improving solar cell performance. National laboratory researchers working in basic and early-stage applied research provide a steady supply of basic science discoveries that feed into the nation's technology development pipeline. The following examples are just a few of the countless contributions that our researchers have made and are continuing to make to enable the energy technologies of the future.

### Saving Billions for American Taxpayers through Energy Efficient Technologies

For more than 50 years, Berkeley Lab has been at the forefront of developing technologies and tools to make buildings and urban infrastructure more energy- and resource-efficient.

Spurred by the energy crisis in the 1970's, Berkeley Lab delved deeply into energy efficiency research, developing many groundbreaking technologies. Particularly impactful is a partnership forged between the Lab, window manufacturers, and the building industry to develop a low-emissivity (low-E), energy-efficient window coating that prevents heat from entering in the summer and escaping in the winter. The technology revolutionized the industry, reducing window energy use by 30-40%. Today, more than half of all residential windows and 80% of commercial windows sold annually have the Low-E coating.

The combined impact of the low-E windows and other Berkeley Lab-developed tools and technologies, including electronic ballasts, simulation software, and appliance standards have saved American consumers more than $484 billion through 2012.

Building on its early research, the Lab continues to drive new innovations in energy efficiency, from individual components to whole building systems. Key to that work is FLEXLAB, the most comprehensive and advanced building efficiency test facility in the world. Used by industry, the public sector, and academia, FLEXLAB allows its users to test energy-efficient building systems individually or as an integrated system, under real-world conditions, ensuring that a building will be as efficient as possible before construction or retrofitting even begins.

With world-leading expertise encompassing lighting, sensors and controls; advanced windows and building envelopes; and simulation and control systems, analytic instruments and computational modeling, Berkeley Lab's uniquely comprehensive portfolio of expertise supports DOE in its mission to develop innovative, cost-effective, energy saving solutions for commercial and residential buildings, ultimately enabling the planning, design, and operation of livable, economically efficient, resilient cities.

**Driving Advances in Energy Storage Solutions**

Energy storage is critical for American energy independence, and Berkeley Lab has a long and successful history of leveraging its scientific facilities and expertise of its researchers to perform world-class, collaborative battery energy storage R&D. With capabilities in materials synthesis and characterization, theory and computational modeling, and design and failure analysis, Berkeley Lab has been at the forefront of game-changing discoveries that have the potential to transform the battery landscape.

In a recent breakthrough, Berkeley Lab scientists collaborated with Natron Energy and New York University to confirm a century-old chemistry speculation, a finding with broad-reaching implications for the future of battery technology. The researchers took advantage of two Berkeley Lab user facilities, the Advanced Light Source and the Molecular Foundry, to study an unconventional, but promising, new sodium-based battery design. They discovered a key to the battery's superlative properties was a novel chemical state of the element manganese. The revelation could lead to new classes of high-performance, low-cost batteries that can quickly and efficiently store and distribute energy produced by solar panels and wind turbines across the electrical grid.

Another example of basic research moving through the technology development pipeline is a porous membrane technology for better batteries. Membranes are an essential component of batteries, and better membrane performance means higher power, greater cycling time, improved efficiencies, and ultimately lower cost. Berkeley Lab researchers affiliated with the Argonne National Laboratory-led Joint Center for Energy Research (JCESR) DOE Energy Innovation Hub developed membranes for lithium-sulfur batteries made from polymers of intrinsic microporosity (PIMs), utilizing the Molecular Foundry and NERSC user facilities. The promise of this basic research to advance toward commercialization became apparent, and the intellectual property for PIMs membranes was licensed by a local startup company, Sepion, to advance the commercialization of this technology, which has also been recognized with an R&D 100 award. Sepion has received support and technology development assistance through the Cyclotron Road program at Berkeley Lab, ARPA-E, and the Advanced Scientific Computing Research-supported HPC-4MFG program. These programs ensure that the most promising advances in technology development are accelerated to market for the benefit of American manufacturing and consumers.

**Lessons from Leaves - Liquid Fuel from the Sun**

An example of an emerging technology that has the potential to transform our energy supply in the future is artificial photosynthesis – a chemical process that replicates plant-based photosynthesis to use sunlight to drive the synthesis of a useful chemical, such as a fuel. This nascent field of research holds great promise for supplying our future energy needs, not just on Earth, but could one day also provide future space expeditions a reliable supply of fuel on the Moon or Mars! Berkeley Lab researchers are pioneering this field in partnership with Caltech through the Joint Center for Artificial Photosynthesis (JCAP), a DOE Energy Innovation Hub. JCAP's first phase was focused on so-called "water splitting"—using a catalyst and the energy from sunlight to extract hydrogen from water molecules to create hydrogen fuel. The basic research discoveries made by JCAP researchers about solar-driven hydrogen generation systems have been transferred to the early stage applied research of the EERE-sponsored HydroGEN Energy Materials Network consortium—an example of DOE's pre-competitive R&D for accelerated commercialization. Meanwhile, JCAP researchers have turned their attention to a new, more scientifically challenging goal of discovering how to produce carbon-based transportation fuels—like the ones we use to fuel today's transportation vehicles— from sunlight, water, and carbon dioxide.