CLIMATE AND ENERGY SCIENCE RESEARCH AT THE DEPARTMENT OF ENERGY

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The Testimony of

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Chairman Bowman, Ranking Member Weber, and distinguished Members of the Committee, thank you for inviting me to testify today and for your interest in materials and chemical sciences research within the Department of Energy (DOE) Office of Science's Basic Energy Sciences (BES) program and its essential role in the development of new technologies and training our nation's scientific workforce. My name is Kristin Persson and I am a Faculty Senior Scientist at Lawrence Berkeley National Laboratory and a Professor at the University of California, Berkeley. My testimony is my own and does not necessarily reflect the views of the U.S. Department of Energy, Berkeley Lab, or the University of California.

It is my pleasure to talk about the Basic Energy Sciences program. BES has been instrumental to my scientific journey and is among the nation's and the world's premier scientific organizations focused on materials and chemical sciences research. BES develops and trains our nation's next generation of scientists by supporting fundamental research at universities across the nation; it supports fundamental science and use-inspired research hubs and science centers at our nation's national laboratories; and it builds and operates some of the world's best and most sophisticated national scientific user facilities, including the Molecular Foundry, where I am the director. The Molecular Foundry is one of five nanoscale science research centers, which are facilities that help envision and realize solutions to today's and future societal challenges by enabling imaging, manipulation and fabrication of materials and chemistry at the molecular and even atomic scale. Scientific user facilities are often large in scale and too expensive for an individual university or company to build and operate, and hence, they offer unique capabilities found nowhere else in the world. Even during a pandemic, over 12,000 researchers or "users" from academia and industry across the nation and the world, and from every U.S. federal research agency, use BES facilities to accomplish their research. Because the operation of these facilities is supported by our federal government, access to them is free of charge for researchers conducting non-proprietary work whose scientific proposals are reviewed well by their peers.

As I will testify below, BES user facilities, unique assets, and expertise are leveraged by hundreds of thousands of researchers from across the country and the world. They empower the nation's inquiry into, and accelerate technology development in, energy storage, quantum information science, transformative new materials and chemicals, artificial photosynthesis, carbon capture at scale, and more.

My personal story sets the stage and illustrates the power of BES and its place in the nation's innovation ecosystem. I immigrated to the US in 2001, and I have raised two daughters here. Today, I am proud to call this country my home as a naturalized citizen. I spent 5 years at MIT before coming to Berkeley Lab, which attracted me with its mission to bring science solutions to the world, specifically with an emphasis on team science and collaborations. This year, Berkeley Lab is celebrating its 90th anniversary and is looking forward to the next 90 with enthusiasm.

Coming to Berkeley Lab, I brought with me a vision of what high-performance computing and quantum mechanical calculations can do for materials innovation, particularly in the energy storage space. I engaged a team of enthusiastic, interdisciplinary researchers to build the first version of a materials data production and online dissemination platform. That vision carried. In 2012, I was awarded one of five DOE-BES Materials Genome Initiative software centers for the platform that my colleagues and I had created - named the ***Materials Project***. Today, the Materials Project is ***the*** world-leading materials data platform. It disseminates millions of computed, pre-competitive materials data records every day to an increasingly data-hungry community of scientists and engineers. This resource is fueling machine-assisted, accelerated learning to the discovery of novel materials with useful properties, and a deep understanding of these materials which will fuel materials design for generations to come.

Since 2012, as the only female principal investigator in the leadership team of the Joint Center for Energy Storage Research (JCESR), a BES Energy Innovation hub led by Argonne National Laboratory, I have implemented a vision of data-driven design for battery materials innovation. In 2020, I became the Director of the Molecular Foundry at Berkeley Lab, one of five DOE BES nanoscale research centers and one of five Berkeley Lab user facilities. And, through my appointment at UC Berkeley, I engage with and teach the next generation of engineers and scientists.

While nearly every aspect of my career has been supported by BES, its facilities, expertise and other research assets have enabled me and many of my colleagues to connect directly to applied sciences helping to advance technology toward applications in society. As an expert in computations, data-driven methodologies, energy storage and materials science, I am regularly called upon to inform industry on the future of battery materials and resources. I have had ARPA-E contracts, and I currently have a broad research portfolio that includes company-sponsored and DOE-EERE sponsored research. In recognition of my contributions, in 2021 DOE-EERE honored me as one of the 23 women who are making significant contributions in energy storage across the national laboratories.

The rest of my testimony will bear witness to the importance of long-term investment in basic energy science research, as a foundation and platform for:

i) Future-looking innovation leadership;
ii) Democratizing the access to knowledge; and
iii) Workforce development.

The Knowledge behind Energy Storage Today and Tomorrow

Today's energy storage technology is built on more than half a century of previous investments in basic energy sciences, which uncovered the details of how ions arrange and move in solid materials. Rechargeable battery materials, where the ions move in and out of the material without greatly changing its structure forms the basis of today's lithium ion (Li-ion) industry.

The materials used today in Li-ion batteries were first studied in the 1970s and 80s at Bell labs, national laboratories, and US universities. As an example, fundamental research to modify the properties of graphite more 50 years ago laid the basis for its uses as a universal anode for Li-ion batteries. Alloying of lithium with main group metals, such as silicon, tin, and aluminum, was investigated in the early 80s as anodes, and today silicon is the focus of major EERE programs as the next-generation anode.

Strong BES programs in materials science, combined with support for investigating the fundamental arrangement of Li ions and their transport mechanisms in solid materials more than 25 years ago, created the insights into fast charging batteries and today's most promising avenues to mitigate nickel and cobalt resource limitations: e.g. novel cation-disordered rocksalt cathodes, recently supported by EERE as an encouraging new direction. The time between fundamental research results and commercial solutions is long – often decades – but the connection is undeniable. Basic energy science research, through the Foundry, the Materials Project, the JCESR Energy Storage Hub, and sister facilities and programs, is driving down the time from discovery to useful technology.

While Li-ion technology has revolutionized our world, it may not be the endgame. To support broad implementation of sustainable energy solutions and retain international competitiveness, JCESR focuses on beyond Li-ion chemistries. Just as decades ago, fundamental research enabled the development of Li-ion batteries, there are today rich and ripe opportunities for building the knowledge at the atomic and molecular scale needed to design the next generation of electrochemical, chemical, and thermal energy storage. For example, high energy density metal-air (zinc, lithium, sodium), multivalent (magnesium^{++}, calcium^{++}, zinc^{++}) and conversion cathode (Li-sulfur) batteries can serve heavy duty and long-haul transportation.

JCESR focuses on these future technologies and uncovers the fundamental bottlenecks in their current state: whether they be limited electrolyte stability or transport limitations in the solid state. The resulting design rules – why certain materials and chemistries work better than others – inform future technological solutions. JCESR leverages BES-funded user facilities such as the Advanced Photon Source (APS) at Argonne, the Advanced Light Source (ALS) at Berkeley Lab, the Molecular Foundry and the Stanford National Accelerator Center (SLAC) to synthesize novel membranes for selective ion transport, and to understand the chemistry of how liquid electrolyte components form clusters which impacts stability and transport. Our ability to 'see' and understand these processes at the molecular and atomic level enables us to devise improvements. One particular limitation comes from the electrochemical stability window of the electrolyte, which impedes the development of high-voltage calcium or magnesium-ion batteries. Because of the sustained and forward-looking investments in JCESR and in other similar basic science programs, ***JCESR has uncovered the fundamental reason why so few calcium and magnesium electrolytes work well, and has now turned that knowledge into a discovery vehicle for the development of new electrolytes with increased stability. We now hold the world record in magnesium and calcium electrolyte formulations.***

The history of fundamental science investments and its connections to today's battery science illustrates the long-term impact of BES science and how it sets the foundation for future technologies.

The Materials Project; Democratizing Pre-competitive Materials Data and Machine Learning

The Materials Project aims to accelerate innovation by removing the guesswork from materials design. Its mission is to compute properties of all known inorganic materials, and beyond, and use structure-chemistry correlations to inspire and design novel materials for applications such as better batteries, affordable carbon capture at scale, and advanced medical diagnostics. Leveraging Office of Science computing and networking resources at the National Energy Research Scientific Computing Center and the Energy Sciences Network, both at Berkeley Lab, we deliver this data to the broad, global community of scientists and engineers using modern web-delivery methods, similar to those used by Google and Amazon. Imagine that Google was more than a sophisticated search engine, collecting, organizing and delivering third-party data. Imagine that it also physically measured, for example, all the traffic, commercial, social, and weather data it showed. That would be the Materials Project; we produce all of our data, organize it, disseminate it, and showcase the design of novel materials for energy applications.

This free access to an enormous and constantly expanding amount of materials data is a new and unprecedented resource. To give an example, the measured elastic tensor, a critically important property for any technology that involves materials, describes how a material deforms under external strain and stress. Any structural design, from bridges to durable solar cells, requires such information. Despite its importance, the complete elastic tensor can be found for only a few hundred materials in the open literature. Using computations and supercomputers, the Materials Project has calculated over 14,000 elastic tensors, which would have taken decades and millions of dollars by traditional synthesis and measurement techniques. The elastic data alone have enabled our own scientists as well as community scientists to use machine-learning algorithms to correlate crystal structure and chemistry to extraordinary elastic behavior, resulting in novel waste-heat capturing materials, super-strong materials, and sound-absorbing materials that could be used in better transportation, building, and energy-saving technologies. The elastic tensor data set shows the impact of allowing free access to the data from ***one*** materials property across structure and chemistry. The Materials Project allows access to millions of such property data points, from materials stability to battery and capacitor metrics such as voltage, energy density and ionic mobility. As a result, novel materials are being realized, aided and accelerated by this novel resource, and every day, one paper is published mentioning the Materials Project and machine learning.

By all metrics, the Materials Project has been a tremendous success. Our audience has been growing exponentially since 2012, and is now approaching 200,000 registered users. Even more importantly, up to 45 million data records are requested and delivered daily, and tens of thousands of community researchers login to the site every day. Allowing free access to high-value, pre-competitive materials data enables diverse minds and innovators across the world to train machine learning algorithms and develop novel materials for sustainable energy production and storage, for climate change mitigation, for waste heat recovery, for energy-smart building materials and more.

The Materials Project represents an example of how BES science democratizes knowledge, data and accelerates learning across communities, without borders.

The Molecular Foundry; a knowledge-based user facility

I am also tremendously proud to represent the Molecular Foundry, home to one-of-a-kind instruments and world-class experts that span the broad field of nanoscale science. As mentioned earlier, the Foundry is one of five BES Nanoscale Science Research Centers. In the simplest terms, nanoscale science is the study of the very small. Because it involves interacting with the world atom by atom, it encompasses every field of science and its impacts are found in every corner of modern-day life. Unlike other facilities centered around billion-dollar machines, the NSRCs are knowledge-based centers for interdisciplinary research at the nanoscale, where access to leading expertise is as important as access to state-of-the-art instrumentation.

Being a user facility, the broad collection of elite capabilities at the Foundry and other NSRCs enable user-driven science that has and will continue to change the world. Our users are visiting researchers who apply to the Foundry through our peer-reviewed proposal process. They come to us from across the country and around the globe, to use our tools and collaborate with our staff. We partner with these users to enable and amplify the impact of their research. Imagine a highly creative early career professor at a remote teaching college or a startup company developing a high-tech device. In both these cases, their great ideas may be hampered by insufficient access to cutting edge scientific tools and world-class experts. At the Molecular Foundry we provide these critical resources, free of charge, to ensure that every good idea has a chance to be explored to the benefit of these researchers, the broader scientific community, and the nation.

Each year, the Foundry supports roughly 1,000 users. They include academics and national laboratory scientists, but also a significant number of industry researchers, most of whom are at small businesses, who use our research infrastructure to de-risk their ideas and build a stronger scientific foundation for their companies. On average, after just a year with us, these industrial users each report that their work at the Foundry results in 1.2 pieces of IP, 3.3 jobs created, and nearly $2M raised.

To illustrate the broad and long-lasting reach of our user model, I will describe some discoveries involving electron microscopy, which is just one of the many areas of expertise found at the Molecular Foundry. In the field of electron microscopy, the

Molecular Foundry's elite tools and expertise provide world-leading capabilities to the scientific community and the nation. The Foundry's TEAM microscopes are two of the most powerful electron microscopes in the world and their development ushered in a new era of science by allowing researchers to study the world atom by atom. The TEAM 0.5 microscope is the product of a multi-institution, industrial collaboration funded by BES. It was the first microscope capable of imaging individual atoms with the resolution of half an Ångstrom, which is the size of the radius of a single hydrogen atom. It was the best microscope in the world when it was completed in 2009, and today, over a decade later, it remains a critical resource for the scientific community. Through the Molecular Foundry's user program, researchers benefit from access to the actual microscope as well as the scientists who are experts at operating it. The unprecedented detailed information of materials has helped unlock fundamental understanding that is critical for future advancement in a range of areas, everything from quantum technologies to learning about the origins of the universe. In the following, I will provide a few examples illustrating the broad and diverse scientific impact of electron microscopy at the Foundry.

Recently, researchers funded by the Toyota Research Institute came to Berkeley Lab with the goal of scanning an entire working battery at the atomic scale. They sought to use the TEAM 0.5 microscope and the 4DCamera, a recently invented camera for electron microscopes that can take pictures at nearly 100,000 frames per second. Using a technique called 4D-STEM, they were able to get atomic scale clarity of the arrangement of atoms inside a battery before, during, and after battery cycling. After the researchers obtained their structural information from the Foundry, they literally walked their samples over to the Advanced Light Source, another BES-supported user facility at Berkeley Lab, and used the X-ray beamlines there to image the distribution of lithium inside them. The synergy of expertise at these two co-located BES user facilities afforded the researchers a complete picture of how the structure of the battery material responds to the movement of lithium ions, which in turn tells us the long-term degradation of these materials, and therefore the battery performance.

A different group of users funded by the U.S. Office of Naval Research accessed a suite of advanced electron microscopes at the Foundry, to understand the role of impurities in titanium for transportation and infrastructure applications. Titanium has the highest strength to weight ratio of any element, but one of the limiting factors for its more widespread use in aerospace, naval and other structural applications is its sensitivity to impurity elements, especially oxygen. Minute amounts of oxygen as low as 0.1 atomic percent can have a profound impact on titanium's structural properties, and minimizing oxygen during processing of titanium is the main driver of its relatively high cost. Using the Molecular Foundry's expertise and advanced imaging techniques, the researchers identified the origins of the profound oxygen poisoning effect, which has also led to identification of mitigation approaches including processing and the addition small amounts of other elements, such as aluminum. Over the years, this project has involved the training and education of multiple generations of graduate students and postdoctoral researchers from different parts of the country, many of whom have now moved on to industry and academia.

These two examples show what world-unique microscopes can do in two dimensions, but we can also image and map atoms in 3D using a special holder that can rotate the sample 180 degrees left and right. It works like a medical CAT scan, taking pictures of a material from multiple angles, that can be stitched together into a 3D image. In 2017, a research team that included UCLA, Oak Ridge National Laboratory, and the United Kingdom's University of Birmingham used the TEAM microscope to image every single atom in an iron-platinum nanoparticle, a material that is magnetic. The ability to create a 3D image of the particle allowed the researchers to explore the different atomic arrangements and thus, different amounts of magnetism. Applications like next-generation hard disk drives for data storage need materials that are highly magnetic. What the TEAM microscope showed was that this material is only 60% magnetic, which is insufficient for this application, but you would not know about the problem without looking at the material atom-by-atom. Now that we can image where all the atoms are and can correlate that to how the material performs, we can work with our chemists to optimize the chemical composition to maximize the ideal atomic arrangement for maximum performance.

The Molecular Foundry exemplifies how BES-funded science democratizes both expert knowledge and high-value instrumentation enabling a broad spectrum of today's breakthroughs and contributing to the next-generation workforce development.

I hope these examples illustrate the many vital roles that BES science plays in the US innovation ecosystem. Without sustained investment in basic materials and chemical sciences, I believe we shortchange and stall technological advances so necessary for our future generations. In my career, I have witnessed the translation of basic research into the applied sciences and further onto viable technologies. BES science creates a fertile platform for exploratory, pre-competitive scientific knowledge, which can be shared and discussed across diverse interest spheres, people and outlooks. The BES-funded user facilities welcome anyone with a great idea to come and work together to solve our current challenges in global warming, sustainable energy production and storage, fresh-water and energy equity. Passionate students, small-businesses, Fortune 500 companies, and academics from every part of the US and beyond, join us, share their knowledge, learn and become part of the global scientific and engineering community striving to improve our world.

Thank you for inviting me to testify. I look forward to answering any questions that you may have.

Kristin Persson obtained her Ph.D. in Theoretical Physics at the Royal Institute of Technology in Stockholm, Sweden in 2001. She is currently a Professor in Materials Science and Engineering at UC Berkeley with a joint appointment as Faculty Senior Scientist at the Lawrence Berkeley National Laboratory where she also serves Director of the Molecular Foundry. Her expertise is materials informatics, specifically pursuing novel and optimized materials for clean energy applications. She has published more than 200 papers in peer-reviewed journals, holds several patents in energy applications, and is among the world's 1% most cited researchers. She is most known for her stewardship of the Materials Project (www.materialsproject.org); one of the most visible of the Materials Genome initiative (MGI) funded programs attracting >180,000 users worldwide with more than 10,000 unique users accessing the site every day. She is a leader in the MGI community, and she serves as an Associate Editor for Chemistry of Materials, on advisory boards of a number of organizations such as NanoHub, FAIRMat, Q4Climate, and various journal editorial boards. She has received the 2018 DOE Secretary of Energy's Achievement Award, the 2017 TMS Faculty Early Career Award, the 2020 Falling Walls Science and Innovation Management Award, the LBNL Director's award for Exceptional Scientific Achievement (2013) and she is a 2018 Kavli Fellow.