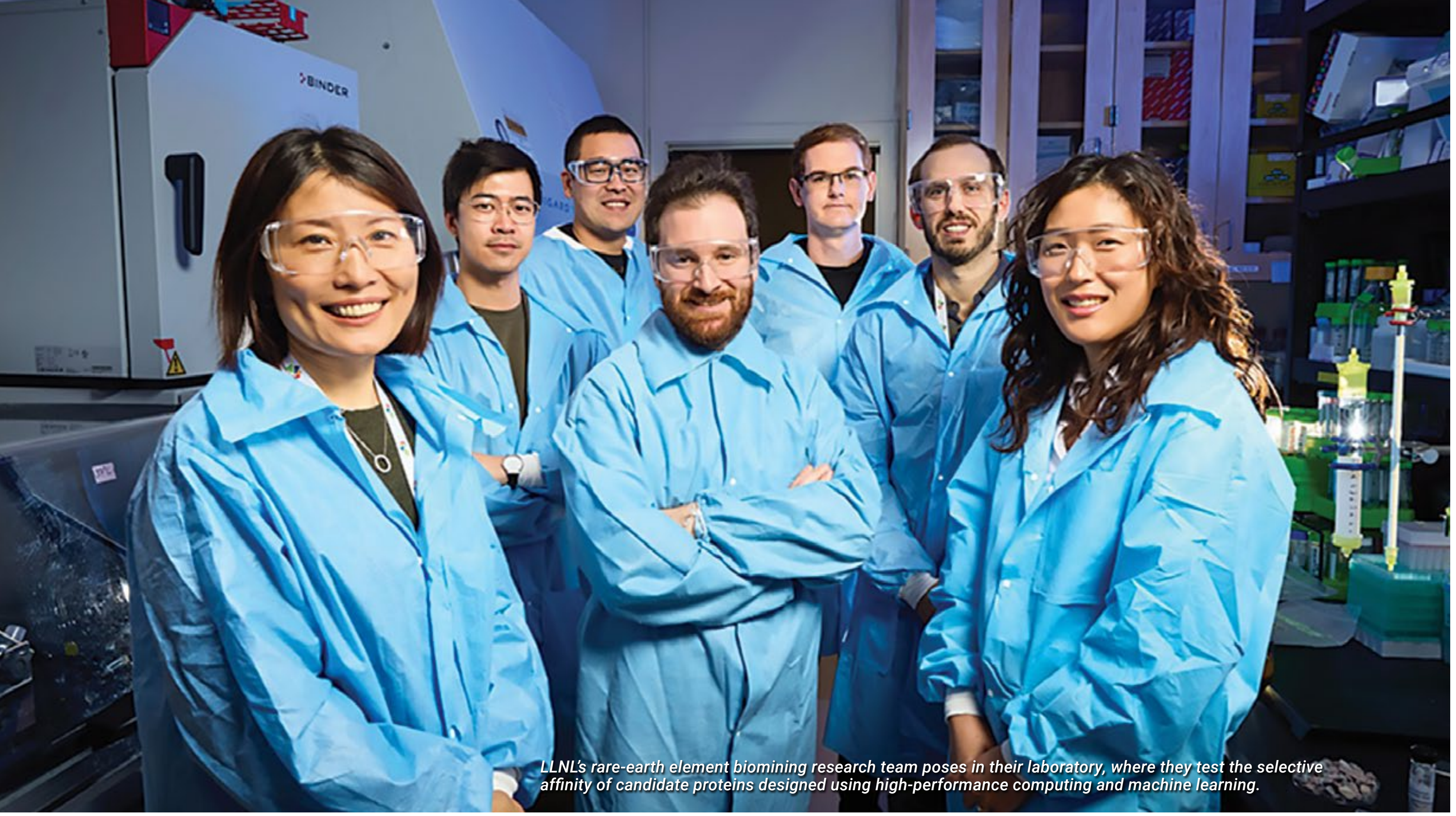


LLNL's rare-earth element biomining research team poses in their laboratory, where they test the selective affinity of candidate proteins designed using high-performance computing and machine learning.

ENERGY AND ENVIRONMENT

Applying science and technology to improve national energy security, protecting the environment and providing for U.S. economic competitiveness

RARE-EARTH ELEMENT SECURITY

Rare-earth elements (REEs) are essential for many electronic, energy, and advanced defense technologies as well as permanent magnets in cell phones. Establishing a domestic supply chain is a national security priority since the U.S. imports more than 80 percent of its REE from offshore, primarily from China, which controls over 95 percent of REE refining. An LLNL–Pennsylvania State University (PSU) research collaboration has generated a portfolio of intellectual property on using bacterial proteins to pick out critical metal ions. The developed biomining technique, called Lanmodulin-Based Earth Purification (LanPure), offers impressive advantages in selectivity, speed, reusability, and sustainability. The currently used chemical processes to extract and purify REEs are complex and harmful to the environment.

Through a licensing agreement with Alta Resource Technologies, an advanced biochemistry start-up company, LanPure is being developed for use at scale. It is a groundbreaking technology that enables highly selective extraction and separation of REEs from diverse sources, including rare-earth ores, mining waste, coal byproducts, and recycled electronics. LanPure builds on a long history of bio-REE extraction process development by LLNL through the DOE Critical Materials Institute. In 2018 researchers at PSU discovered the lanmodulin (LanM) protein. LLNL and PSU jointly originated concept of LanPure; LLNL developed it using LanM's strong ability to selectively bind to REEs and achieve high-purity separations. LLNL–PSU research efforts continue, using LLNL's high-performance computing (HPC) and machine learning (ML) capabilities to design proteins that enhance REE specificity and affinity as well as proteins that would effectively separate other critical metals.

ENHANCING THE ENERGY GRID

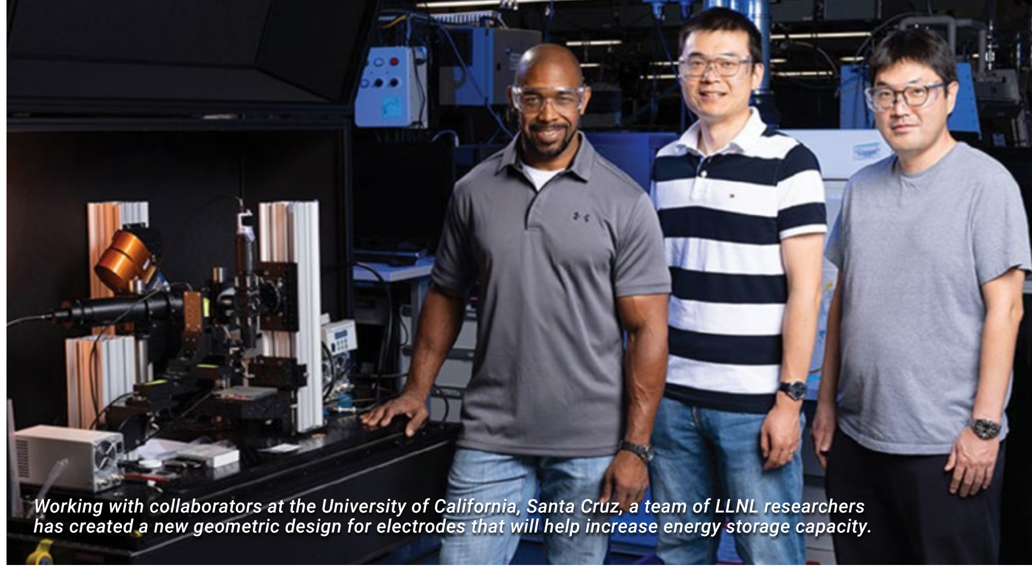
Livermore applies its expertise in HPC simulations, uncertainty quantification, risk analysis and decision support, and data analytics and ML to advance power grid modeling and enable resilient grid design and operations. LLNL researchers support DOE's grid modeling efforts by developing and, importantly, improving the performance of HPC modeling capabilities that integrate transmission and distribution components of the grid. In FY 2025, the use of AI to augment these modeling tools enabled the Laboratory to undertake high-impact projects for sponsors that have the potential to improve the safety, reliability, efficiency, and resiliency of the nation's power grid and protect the nation's critical infrastructure. Research included efforts to build next-generation "early warning and response" systems for cyber attack protection (see pp. 10–11).

In one study, reconductoring–replacing existing power lines with new conductors to increase capacity or improve performance—was examined as a response option to the stress on the energy grid posed by the rapid proliferation of large power-consuming AI data centers. Could it help? How much incremental new generation could be avoided and at what cost? LLNL researchers used detailed models of California's grid, identified suitable reconductoring corridors, and found that the option would obviate the need for 17.5 gigawatts of new generation (about half the projected total) and avoid $1.5 billion annual congestion costs. A lower resolution survey of other regions of the nation identified those that would benefit from a comparable analysis.

BETTER BATTERY DESIGNS

Electrodes with increased surface area and storage capacity make possible next-generation electrochemical energy storage devices (EESDs). Conventional thick electrodes limit reaction kinetics and storage capacity. LLNL scientists and collaborators at the University of California, Santa Cruz performed computer simulations to design and then 3D-print a new compact device configuration with two interpenetrated, individually addressable electrodes. The design improves ion-diffusion kinetics in EESDs. The researchers used a zinc manganese dioxide battery as a model system and found that the device outperforms conventional separate electrode configurations, improving volumetric energy density by 221 percent and exhibiting a higher capacity retention rate. This new EESD architecture is applicable to lithium-ion and sodium-ion batteries, supercapacitors, and other storage systems.

Another LLNL research team modeled in detail a multiphase material typically used in all solid-state batteries.



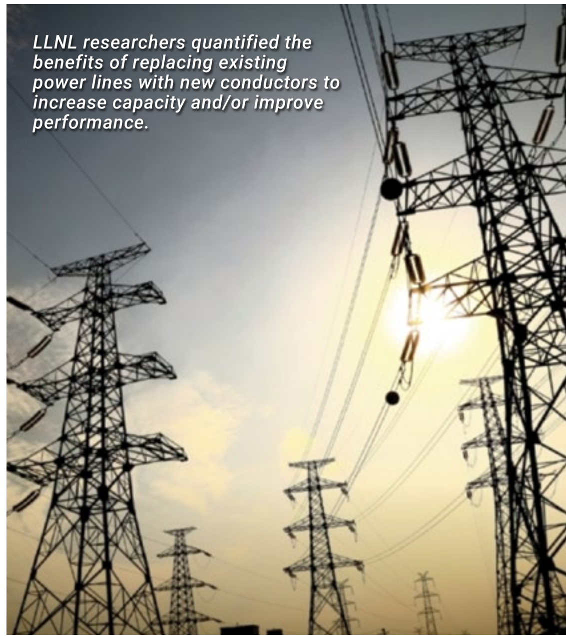
Working with collaborators at the University of California, Santa Cruz, a team of LLNL researchers has created a new geometric design for electrodes that will help increase energy storage capacity.

They developed a computational framework able to identify and improve key interface and microstructural features in materials to increase ion diffusivity—how quickly and efficiently a battery can charge and discharge. Their framework employs a new method for generating many digital representations of distinct material microstructures with different grain, grain boundary, and interface configurations. The microstructural data was then used to train a mesoscale machine-learned model, which is able to pinpoint specific microstructural features that critically affect effective ionic diffusivity. The modeling framework can be extended for understanding generic microstructure–property relationships in other complex multiphase materials.

PUTTING CO_2 TO WORK

Combining additive manufacturing (AM) with multiscale modeling, Livermore researchers are rapidly cycling the design and testing of modular electrochemical reactors with enhanced performance. An important potential application is the conversion of carbon dioxide (CO_2) into ethylene, the most common carbon-based commodity chemical in the world. Yet, to date, CO_2 electrochemical reactors have been limited by their low efficiency, which makes them too energy-intensive for wide application. To meet this challenge, LLNL researchers designed a new polymer ink, called an ionomer, that controls how gas and water move in electrochemical devices. By carefully balancing and directing the device chemistry, the ionomer improves energy efficiency of the conversion process. Inside the device, CO_2 encounters a copper catalyst layer that triggers a reaction to turn it into ethylene. The ionomer, which is sprayed as a coating onto this copper layer, controls the chemistry of the catalyst surface and ensures that the right amount of water and CO_2 reach the catalyst.

In another study, LLNL researchers explored how a reactive CO_2 capture and conversion (RCC) process could be used to produce synthetic renewable natural gas. Solar and wind energy are highly variable, at times generating electricity that can be used to separate hydrogen (H_2) from water. The RCC process uses a dual-function material with the chemical components to first capture CO_2 and then to react it with H_2 to produce methane, a main component of synthetic natural gas. The research team found that, in many cases, the RCC process is less expensive than other utility-scale long-term energy storage solutions. Experimental teams at LLNL are working to develop the dual-function material, demonstrate the proposed RCC process, and partner with industry to scale up the technology.



LLNL researchers quantified the benefits of replacing existing power lines with new conductors to increase capacity and/or improve performance.