PHYSICAL SCIENCES

VISTAS

PERSPECTIVES ON SIMULTANEOUS EXCELLENCE | ISSUE 2 2023

INSIDE

Los Alamos NATIONAL LABORATORY

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← On the cover: A photo illustration depicting improvements to the Proton Radiography Facility, which were the result of teamwork between the Lab's scientific and operations staff.

Physical Sciences Directorate

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The Chi-Nu project, a years-long experiment measuring the energy spectrum of neutrons emitted from neutron-induced fission, recently concluded the most detailed and extensive uncertainty analysis of the three major actinide elements—uranium-238, uranium-235, and plutonium-239. The results have contributed essential, never-before-observed data for enhancing nuclear security applications, understanding criticality safety, and designing fast-neutron energy reactors. The Chi-Nu apparatus, located at the Weapons Neutron Research Facility at the Los Alamos Neutron Science Center, includes 54 liquid scintillation neutron detectors and 22 lithium-glass detectors to measure neutrons in different energy ranges.

FROM ELLEN'S DESK

Ellen Cerreta, Associate Laboratory Director for Physical Sciences

Happy New Year!

I was pleased to see so many from the directorate attend our all hands to close out fiscal year (FY) 2023 and hear about so many of our big achievements. Not surprisingly, many of the highlights included successes in developing new capability for the Laboratory. Whether it was installing the new 1L target at the Los Alamos Neutron Science Center (LANSCE), achieving Hazard Categorization 3 in the RLUOB (Radiological Laboratory Utility Office Building), or completing an overwhelming 33 construction projects in the Sigma Complex, it was delightful to be reminded that while sometimes executing large projects can be challenging—we, as a Laboratory, can successfully imagine and implement new capability.

In addition to that, and as one of the primary work execution organizations at Los Alamos, we had many scientific and engineering achievements this year, some of which are highlighted in this *Physical Sciences Vistas* issue. In addition to this, and an achievement that I have highlighted to the Lab Director, is that we had an incredibly large number of awards presented to our folks for their work. I am looking forward to this year's awards recognition night that the Lab Director will hold in late October to celebrate our LANL award winners. Moreover, for those that feel like sometimes classified work does not get the same attention, you will be glad to know that this fall's Triad Science, Technology, and Engineering committee meeting will be focused on achievements by our colleagues behind the fence. I am looking forward to that meeting and already am trying to consider how we might share those talks beyond the limited attendance of the Triad meetings.

Of course, the new fiscal year is also bringing some significant change. Uncertainty in budgets, getting to know an interim Deputy Director for Science, Technology, and Engineering, start up for the beam cycle at LANSCE, and management of the mortgages we carry into the new year for big projects like Plutonium Facility (PF)-4 Equipment Installation-Phase 2, the Low Enriched Fuel Fabrication Facility, and the rotor at the National High Magnetic Field Laboratory-Pulsed Field Facility are only some of the topics that consume many of our thoughts right now.

At the same time, this is creating a new energy at the Lab. I am seeing novel ideas emerge for more efficient operational modes, enhanced support amongst the collective leadership team for the health of LANSCE, and a really energizing effort around revamping the Lab Agenda and how we use it to guide our work. So, in those ways, I am really looking forward to the new year and seeing what all of our hard work will enable for our national security mission.

As always, I look forward to hearing from all of you and am hoping to continue to expand my knowledge of your work and how I can help in the new FY.

Ingenuity, collaboration enable mission-essential work and improved operations

When a hazard analysis revealed that the Proton Radiography Facility (pRad) was operating under an inaccurate building code, mission-essential work threatened to grind to a halt. The facility uses protons from the Los Alamos Neutron Science Center (LANSCE) accelerator to study the behavior of materials driven by high explosives, providing vital data—unattainable through other means—to NNSA Defense Programs.

However, thanks to close collaboration between members of the Lab's scientific and operations staff, a safe and efficient course of action was defined that allowed critical research to continue while a permanent solution was established.

The improvements bring the facility into compliance with its high-hazard building code, allow a mission-essential program to get underway, and strengthen the safety environment for those working in pRad and the adjacent Ultracold Neutron Facility (UCN).

Hazard requirements present a challenging task

"The Proton Radiography Facility is in the unique situation of handling three separate facility hazards: fire, radiation, and high explosives," said Accelerator Operations and Technology (AOT) Deputy Division Leader Mark Gulley, who noted these hazards can have conflicting requirements.

Upon discovery of the situation, operations were immediately paused. Working with the Los Alamos Site Office, line management and LANSCE Facility Operations (LANSCE-FO) developed a safety plan that temporarily allowed experiments using high explosives to proceed. Within days, pRad was back in action, albeit with emergency responders on standby during experiments and additional constraints during high explosive handling operations.

continued on next page ▶

A new elevated walkway traverses the accelerator beamline, providing improved egress from the Proton Radiography Facility during the run cycle.

Additional lighting makes the shielding tunnel easier to navigate.

Ingenuity, collaboration continued ...

"Good near-term and long-term solutions to the code compliance issues were identified as a result of LANSCE personnel working closely with the Lab's Fire Marshal and the Los Alamos Field Office's fire protection subject matter expert," said LANSCE-FO Director Charles Kelsey.

Timely work execution supports mission-essential deliverables

For a lasting solution, the requirements for pRad to operate as a high-hazard facility were determined and promptly implemented. This included installing new fire detection systems, emergency lighting, and an elevated walkway over the beamline and replacing mesh fencing with a solid firewall. An existing door in pRad's six-foot-thick concrete blast shield was enlarged, allowing workers to move larger components in and out of the experimental area during operations.

"The work's completion, before the start of the 2023 LANSCE run cycle, was critical as we prepare to start small-scale dynamic experiments using plutonium at pRad," said Dynamic Imaging and Radiography (P-1) Group Leader Keith Rielage. The "Pu@pRad" program is the culmination of several years' worth of effort to undertake such experiments as a complement to large-scale experiments at the Nevada National Security Site.

Future enhancements to benefit fundamental, applied science

Further improvements are planned that will benefit research at both pRad and the adjoining UCN. UCN uses the LANSCE beam to produce the world's highest density of ultracold neutrons for fundamental nuclear and particle physics experiments. Significantly, the enhancements will enable UCN to operate while the pRad dome is occupied, which is currently not possible due to the configuration of a shared beamline. The result will be more experimental beam time for UCN during pRad set-up activities. ■

Organized cable racks give a visual representation of the complex design, planning, and installation effort required to bring the Proton Radiography Facility into compliance with its high-hazard building code.

Get the details

The work was a collaborative effort between members of Accelerator Operations and Technology (AOT); LANSCE Facility Operations (LANSCE-FO); Physics (P); Acquisition Services Management (ASM); Engineering Services (ES); Logistics (LOG); and Occupational Safety and Health (OSH) divisions; and the Infrastructure and Capital Projects Directorate (ALDICP); in addition to subcontractors Pueblo Alliance; Pueblo Electric; and RG Construction Services. The Weapons Infrastructure Program Office funded the majority of improvements, which support NNSA Defense Program missions. *Technical contact:* Keith Rielage

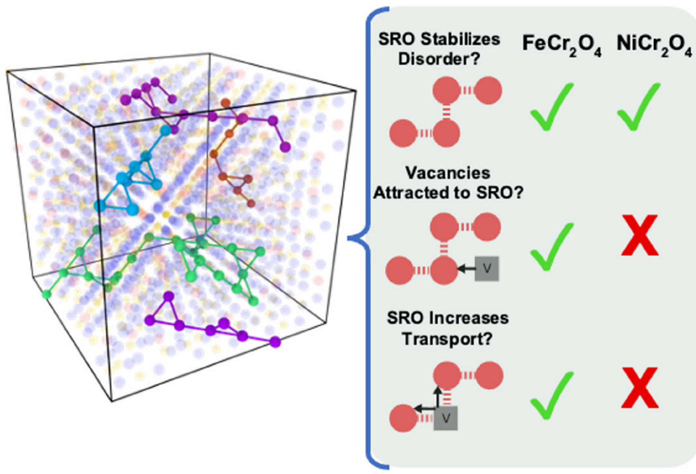
Understanding short range order in **disordered spinels**

Work furthers efforts toward advanced energy materials

Spinels are important complex oxides used in radiation damage environments such as nuclear reactors and which can also result from the corrosion of steel. In radiation damage environments, spinels exist with some concentration of cation antisite pairs, resulting in a modification of the material's chemical order known as "inversion." A spinel's ability to accommodate this inversion process is a key aspect of its resilience in radiation damage environments.

In work published in the *Journal of Materials Chemistry A*, Peter Hatton and Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8) showed that even in highly disordered states characterized by high levels of inversion, spinels exhibit a high degree of short range order (SRO) that manifests itself in antisite chains. This resulting structure modifies defect transport, thus affecting the material's performance.

The work furthers efforts to understand defect transport in these disorder materials, which is necessary to describe, predict, and control the material's properties, and ultimately its performance.



Left: An illustration of the development of short range order (SRO) in disordered spinels as might form under irradiation. The SRO manifests as linked antisite chains, indicated by the highlighted atoms. Right: Metrics used to understand thermodynamic and kinetic effects of SRO, which are chemistry dependent. In $FeCr_2O_4$, the result of SRO is enhanced transport. In $NiCr_2O_4$, the SRO increases the transport of some species and slows that of others.

Examining materials in harsh service conditions

The work was supported as part of FUTURE (Fundamental Understanding of Transport Under Reactor Extremes), an Energy Frontier Research Center funded by the DOE, Office of Science, Basic Energy Sciences.

FUTURE Director Uberuaga said the center is dedicated to understanding how the extreme conditions encountered by materials in nuclear reactors—radiation damage, corrosive environments, high stresses, and high temperatures—couple to impact the properties of the material, with the goal of understanding how the material will evolve.

Disorder in spinels induced by radiation damage was simulated using a Metropolis-based Monte-Carlo procedure. The thermodynamic properties of chain-based SRO were probed using atomistic modeling for different chemistries. Thermodynamic and kinetic properties of vacancy defects in environments of SRO were investigated using molecular dynamics simulations.

These simulations revealed that SRO impacts transport differently depending on the chemistry of the spinel, significantly enhancing it in some, highlighting the need to carefully examine the properties of each individual material. The work leveraged the Laboratory's expertise in the modeling of both defect transport and complex oxides. ■

Get the details

The work supports the Laboratory's Energy Security mission and Materials for the Future capability pillar, particularly its science themes of Defects and Interfaces and Extreme Environments—by probing pathways to developing materials with controlled functionality and predictable performance, the key aim of the Lab's Materials for the Future strategy. Reference: "Short range order in disordered spinels and the impact on cation vacancy transport," *J. Mater. Chem. A*, 11, 3471-3480 (2023). Authors: Peter Hatton and Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8). *Technical contact*: Blas Uberuaga

New design for high-power-density fuel cells offers **improved performance, durability**

Promising new hydrogen fuel cell technology, developed by a team of Lab materials scientists and external colleagues, has up to 50% higher performance than current, state-of-the-art technology, with improved durability. The grooved electrode design advance may help optimize next-generation fuel cell technology to power emission-free medium- and heavy-duty transportation.

"We had a theory that by reimagining the way electrodes are designed we could achieve improved performance," said Jacob Spendelow (Materials Synthesis and Integrated Devices, MPA-11), part of the team that described its results in *Nature Energy*. "One of our biggest takeaways is that novel materials are not the only route to improve performance. The way the materials are put together can be equally important."

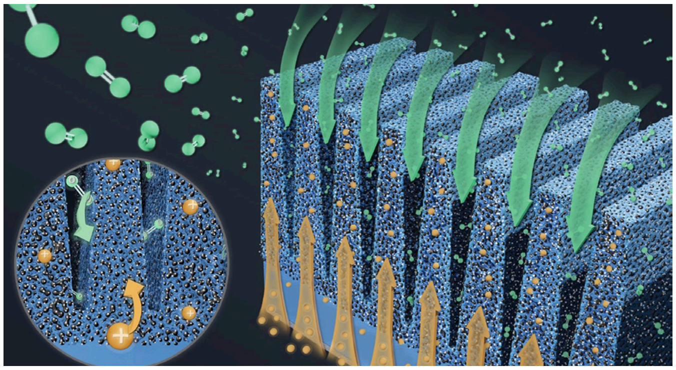
"All we did was take conventional commercially available materials and change the way we put them together to change the microscale architecture, and that resulted in substantially higher performance."

Hydrogen fuel cells—and specifically a version of the technology called proton exchange membrane fuel cells—represent an emission-free engine design that uses hydrogen as a fuel. Fuel cells could transform the medium- and heavy-duty transportation sector, which has been difficult to decarbonize.

Design promotes efficiency and durability

In a fuel cell device, hydrogen and oxygen are reacted electrochemically to produce an electric current capable of powering an external device, such as an electric motor. The electrochemical reactions occur within the fuel cell electrodes, which include a platinum-based catalyst to enable the reaction and an ion-conducting polymer (ionomer) to transport the protons needed to complete the reaction.

Spendelow and colleagues developed a grooved electrode design that improves the efficiency with which oxygen and protons are transported through the device. The team fabricated the device at the Lab's Center for Integrated Nanotechnologies, using photolithography and deep reactive ion etching at the micrometer scale to pattern silicon templates for electrode fabrication. The resulting electrode consists of catalyst ridges with high ionomer content separated by empty grooves, which protons and oxygen use as pathways to more efficiently move through the system. The team's diagnostics, combined with multiphysics modeling and simulations, demonstrated the improved oxygen transport. Machine learning also offered opportunities to guide the calculations of the multiphysics modeling, saving computing time. Notably, grooved electrodes also improved durability, even after carbon corrosion.



The grooved electrode design enables the transport of oxygen and protons to be partitioned into separate grooves and ridges, respectively, enabling faster movement of both species, and hence higher fuel cell performance. First published in *Nature Energy*, 2023, by Springer Nature.

A history of innovation

The original fuel cell membrane electrode assembly was invented at Los Alamos more than 30 years ago, but the fuel cell design used today has barely changed, Spendelow said. "This grooved electrode is one of the first alternative electrodes that can replace the historic Los Alamos electrode."

The fuel cell team will continue to develop the grooved electrode design, especially looking to engage with manufacturing-specific research and development. Scaling up the fabrication to deploy it in a roll-to-roll manufacturing facility, with high-speed and low-cost manufacturing, is a long-term goal. ■

Get the details

The work was supported by the DOE Office of Energy Efficiency and Renewable Energy's Hydrogen and Fuel Cell Technologies Office, through the Million Mile Fuel Cell Truck (M2FCT) consortium; the Los Alamos Laboratory Directed Research and Development Program; and DOE Office of Science funding of the Center for Integrated Nanotechnologies and the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory. Reference: "Grooved electrodes for high-power-density fuel cells," *Nature Energy*, 8, (2023). Researchers: Tanvir Alam Arman, Rod L. Borup, Jacob S. Spendelow, Siddharth Komini Babu (Materials Synthesis and Integrated Devices, MPA-11); ChungHyuk Lee (MPA-11, Toronto Metropolitan University); Wilton J. M. Kort-Kamp (Physics of Condensed Matter and Complex Systems, T-4); Haoran Yu, David A. Cullen (Oak Ridge National Laboratory); Brian M. Patterson (Engineered Materials, MST-7); and Rangachary Mukundan (Lawrence Berkeley National Laboratory).
Technical contact: Jacob Spendelow

Creating novel materials through innovative **metal spray technology**

Spray painting is a relatively simple and versatile technique. Pressing the spray can's nozzle releases a stream of tiny droplets directed at a surface to be coated. Moving closer to the surface creates a smaller and thicker coating. Moving farther away creates a larger and thinner one. Using this technique, an expert artist can create complex, thought-provoking images. For example, murals created by the British street artist Banksy are sought out by admirers and his screen prints can fetch six figures at auction.

At Los Alamos's Sigma Complex, comparable techniques with metal materials are used in support of the Lab's national security mission. For decades, Sigma researchers have employed metal spray technologies to create both protective and functional metal coatings for wear control and corrosion and oxidation protection.

Now, thanks to innovations in spray technology, functionally graded coatings—novel materials that combine the characteristics of the raw ingredients to produce new or unusual properties—are possible. New thermal spray instruments can increase deposition control and the density of the sprayed material. These advances hold promise in solving a range of challenges in engineering and industrial applications, particularly for materials subjected to extreme conditions.

To leverage these technological improvements and meet increased demand for the technique, Sigma researchers are introducing new equipment to their toolkit. The hardware replaces a single, home-built plasma spray unit, housed in the facility's basement, which was used to deposit metal on simple surfaces.

Located at the end of a robotic arm, the cold spray system's applicator nozzle (shown in the image above at lower left) is used to produce metallic coatings.

The thermal spray system's vacuum chamber contains equipment for depositing coatings of reactive feedstock or substrate materials.

Modernizing and increasing flexibility

For the first time, cold spray technology is being introduced to the Lab in the form of a new system that deposits multiple types of feedstocks in atmospheric conditions. The US Navy makes heavy use of this equipment for repairing damaged surfaces and to assist in dissimilar metal joining. "Los Alamos plans to use this equipment for dissimilar metal joining as well, but is putting its own national laboratory 'spin' on it," said John Carpenter (Finishing Manufacturing Science, Sigma-2).

As part of the Laboratory Directed Research and Development (LDRD)-Directed Research project DOGMA (for Design of graded metal arrangements to improve producibility), Lab researchers are exploring using cold spray to create compositionally graded interfaces. Unlike two separate metal components, these graded interfaces create a single bimetal component, thus greatly simplifying supply chain issues and assembly.

continued on next page ▶

Get the details

Funding sources for this technical work include NNSA's Office of Engineering and Technical Maturation's Advanced Manufacturing Development Program; DOE's Office of Nuclear Energy's Microreactor Program; and the Los Alamos Laboratory Directed Research and Development Program under project number 20230128DR. *Technical contacts*: Kendall Hollis and John Carpenter

Creating novel materials continued ...

As well, cold spray—unlike traditional joining techniques, which apply significant heat and as a result do not always work with all compositions—provides minimal heat. This ensures no melting occurs and instead creates a strong bond through plastic deformation. “So far, the bond’s strength has proved sufficient for a multitude of potential applications,” Carpenter said. “These range from quasi-static loading—think of the stress on an office chair—to dynamic loading—the impact of a car crash.” Carpenter and Saryu Fensin (Center for Integrated Nanotechnologies, MPA-CINT) are the project’s co-principal investigators.

Interested in protective coating methods with a smaller space and environmental footprint for production missions, the Advanced Manufacturing Development Program funds research in cold spray technology. Such units take up only 1 to 2 cubic meters, require only an electric plug, and involve no chemical waste. The new machine can be used for coatings as a form of additive manufacturing to create functionally graded interfaces—as in the LDRD project.

Small footprint, big impact

Sigma’s new cold spray system uses powdered metal particles—often heated to far lower than their melting point—sprayed at high velocity, which causes the particles to deform and “stick” to the surface. Coatings as thin as ~75 μm can be rapidly achieved, with several square feet of surface coated in mere minutes in normal atmospheric conditions. The system is optimal for soft metal materials deposited on harder substrates.

A second, new thermal spray system, housed within a vacuum system, allows coatings with potentially reactive metal powders and metal substrates. Originally intended for use with nuclear fuel, the system is flexible and its technique aids a variety of missions. Coatings with thicknesses as low as ~25 μm are possible. Heat is used to partially melt the material to improve sticking, thus allowing both hard and soft metal feedstocks to be placed on both hard and soft substrates. In addition to protecting reactive materials from the atmosphere, thermal spray creates a porous coating that can create a dampening effect in shock environments, which is important for materials subjected to extreme environments. ■

MEET JACKIE MIRABAL

Deputy Group Leader, Applied and Fundamental Physics, P-2

To all her myriad job duties, Jackie Mirabal brings a passion for uniting people and a focus on safety to achieve a successful outcome.

“I have learned that the people of our organization are the most important part of what makes us all successful,” she said. “I am continuously impressed by the diversity in ideas, commitment to problem solving, and ingenuity demonstrated by staff when working collectively on a shared goal. I value being a part of setting the cadence for the working legacy we all leave for the future.”

As a Physics deputy group leader, Mirabal facilitates the work of experimental physicists, engineers, technicians, and students engaged in a range of nuclear physics research. One day she is connecting people to ensure the safe and steady installation of a new piece of equipment to build new capabilities. The next, she is coordinating resources and subject matter experts to complete pressure safety system corrective actions and policy implementation. She has also built a new professional development program that incorporates career planning for each staff member in her group.

As the science, technology, and engineering requirements and perspective lead on the Lab’s Work Planning and Control Integrated Project Management Team, she is gathering feedback on a software tool to identify and analyze workplace hazards and recommend controls. Her work is part of an initiative to bring a Lab-wide, systems-based approach to consistently integrate safety, security, and environmental requirements into all work practices.

Mirabal, who joined the Lab as an undergraduate student, has 25 years of experience in electronics design, fabrication, and testing. For more than 15 years she was the division’s electrical safety officer and was the first woman to chair the Lab’s electrical safety committee. Most recently she was the division’s safety and compliance coordinator. Prior to that she was the principal investigator for subcritical experiments at the Nevada National Security Site.

“My experience has given me the opportunity to see science experiments from many perspectives,” Mirabal said. “I am grateful to have been a part of an organization that nurtures the creation of new fields of science and engineering, while incorporating operational excellence.” ■

Lab volunteers guide students through hands-on STEM experience

For 36 high school students from across the country—including 7 from New Mexico—this summer offered the opportunity for them to discover their STEM potential, as they worked side-by-side with scientists passionate about their work.

The Joint Science and Technology Institute (JSTI) West, held at the University of New Mexico in Albuquerque, paired Lab volunteers with students who performed hands-on research that ranged from polymer chemistry and bioscience to engineering and materials science.

JSTI is an annual two-week, residential, no-cost program, funded by the Defense Threat Reduction Agency (DTRA) through the Oak Ridge Institute for Science and Education. The institute aims to inspire and engage students in STEM (science, technology, engineering, math) careers, with a particular focus on those from underrepresented communities. JSTI began in Maryland in 2012 and expanded to New Mexico, with Lab support, in 2019.

In addition to science projects, the program also offered students the opportunity to learn about the work of DTRA, the national laboratories, and other government agencies. JSTI West concluded with the students presenting their research projects before family, organizers, and DTRA administrators.

"By involving the students in real time multidisciplinary research projects, we can open their eyes to the wealth of unusual STEM career opportunities found at our national labs and government agencies," said Ricardo Martí-Arbona. The Chemistry acting deputy division leader coordinated this year's program and recruited more than 50 volunteers from the Lab. ■

Students on the "Smart polymer materials that heal themselves" project synthesized polyurethanes—a commonly used polymer material in automotive interiors and furniture—and tested the mechanical properties of the resulting materials. Mihee Kim and Kyungtae Kim (both Center for Integrated Nanotechnologies, MPA-CINT) organized the project that exposed students to the protocols of chemistry and materials science research.

During the two-week program, JSTI West students took part in team building, cultural, and recreational activities, including excursions to the Bradbury Science Museum and the Los Alamos Neutron Science Center in Los Alamos County and the Main Event entertainment center, the BioPark Zoo, Indian Pueblo Cultural Center, and Sandia Peak Tramway in Albuquerque. Here, Jennifer Martinez (Materials Physics and Applications, MPA-DO) talks with students about her career path as a nanoscientist.

In "Reverse cycling," students studied the engineering and material science aspects of the composition of a bicycle helmet. Benjamin Derby and Jesse Callanan (MPA-CINT); Bernard Gaskey (Finishing Manufacturing Science, Sigma-2); and Franziska Schmidt, Aditya Shivprasad, and Sim Kim (Materials Science in Radiation and Dynamics Extremes, MST-8) mentored the team.

Get the details

The JSTI West camp included volunteers from the Materials Physics and Applications (MPA); Sigma (Sigma); Bioscience (B); Computer, Computational, and Statistical Sciences (CCS); Emergency Management (EM); and X Theoretical Design (XTD) divisions. JSTI West provides a two-week residential STEM experience for students ages 16-18 with a minimum GPA of 2.0 from across the country. For more information, please see orise.orau.gov/jstiwest/default.htm. *Technical contact:* Ricardo Martí-Arbona

LANSCE Family Day

Exploring the wonders of science at a particle accelerator

The Los Alamos Neutron Science Center (LANSCE) threw itself a birthday party this spring, and more than 600 participants joined the celebration. LANSCE, which turned 50 recently, opened its doors to friends and family members of those who work on the mesa—the first time in more than a decade for such an event.

The Laboratory values collaborative problem solving, as positive teamwork advances understanding and knowledge and facilitates accomplishment of the Lab's work goals. Here (clockwise from left), materials postdoctoral researchers Darrell Cheu, Maria Kosmidou, Md Mehadi Hassan, and Umanga De Silva take advantage of collaboration space in the Materials Science Laboratory.

Associate Laboratory Director for Physical Sciences: Ellen Cerreta
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