Alkaline earth atoms may hold the key to a new evolution in quantum computing

Propelling Los Alamos to the forefront of next-generation accelerator design

5 steps to a safe, productive, efficient workspace
From Toni’s desk

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9. Yong Wang (left) and Matthew Chancey (both Materials Science in Radiation and Dynamics Extremes, MST-8) align a helium ion beam to a thickness-graded gold foil on the tandem accelerator in the Ion Beam Materials Laboratory. Their results will be used to simulate the alpha spectrum emitting from the surface of plutonium and to conduct material compatibility studies in support of Laboratory science and engineering campaigns and other defense programs.
I am excited to introduce the first 2020 issue of Physical Sciences Vistas, with a focus on “excellence in mission-focused science, technology, and engineering.” Excellence in mission-focused ST&E comprises one of the four elements of the Laboratory Agenda, focusing on sustaining and enhancing LANL’s science base. This issue highlights the diverse efforts of personnel in our Physical Sciences Directorate (ALDPS) to enhance science, technology, and engineering at the Laboratory. As we reflect on work at the Laboratory, mostly from our homes due to COVID-19, it is gratifying to see the important, diverse contributions to ST&E across ALDPS.

In this issue, highlights of our contributions to mission-focused ST&E include descriptions of the following.

• New research in MPA-Q on trapped strontium atoms, cooled to sub-micro-Kelvin temperature, to enable nuclear-spin qubits for quantum information science. This research underpins the Lab Agenda goal of leadership in the national quantum initiative.

• The commissioning of a high-power radio-frequency (C-band) accelerator test facility that will propel the Laboratory to an international leadership position in the development of high-gradient electron accelerators. This AOT Division facility, and the associated LDRD-DR project, supports the Lab Agenda goal of advancing accelerator ST&E, as well as the Nuclear and Particle Futures science pillar.

• Recognition of Abul Azad, a scientist in MPA-CINT, as a 2020 Fellow of The Optical Society for his pioneering work in quasi-two-dimensional metamaterials that enable novel, compact optical devices.

• The successful investigation of spherically imploding supersonic plasma liners at P-24’s Plasma Liner Experiment as a potential compressive driver for magnetized target fusion, with the ultimate, long-term goal of achieving fusion energy.

• A materials co-design effort, merging manufacturing capabilities in Sigma Division with nanoscale characterization in MPA-CINT, and modeling and simulation in MST Division, to control microstructural instabilities with the goal of realizing damage-resistant materials.

• A 2019 R&D 100 Award, “Atomic Armor,” to develop photocathodes with increased quantum efficiency, enabling the development of enhanced electron sources for next-generation accelerators. This award, enabled through a multi-divisional collaboration (AOT, Sigma, T, and C Divisions) supports the Lab Agenda goal of advancing accelerator ST&E, as well as the Materials for the Future science pillar.

In support of excellence in mission operations, ALDPS is actively engaged in the Laboratory’s 5S + Safety initiative to create order in the workplace. The 5S initiative—Sort, Set in order, Shine, Standardize, and Sustain—is led by Christie Davis, Sigma-DO, and Jacki Mang, LANSCE-FO. All five of the steps are critical to changing workplace culture so that our work is easier, less stressful, and more productive.

Finally, we summarize the ALDPS contributions to Science Education Community Service. ALDPS contributed 293 hours of community service in 2019, ranging from contributions to multiple science workshops and mentoring programs to judging science fairs. These outreach efforts by our staff strengthen STEM education throughout Northern New Mexico and LANL’s partnerships with the community. This voluntary engagement is greatly appreciated.

As we continue dealing with the COVID-19 pandemic, I want to thank everyone for their patience and efforts to deal with this “new normal,” in terms of working from home and maintaining social distancing while at the Laboratory. I know this is not easy. Hang in there—we will get through this together!
In the rapidly evolving field of quantum computing technology, the “state-of-the-art” is difficult to define. The term could be claimed for systems of trapped ions, superconducting qubits, or neutral alkali atoms, among other approaches for harnessing the laws of quantum mechanics to build machines that far surpass the processing power of conventional computers.

Nevertheless, demand is growing for access to new and varied “noisy intermediate-scale quantum” (NISQ) hardware, as each approach offers its own strengths and weaknesses—a variety that enriches fundamental research in this field. Access to these NISQ systems paves the way for solving complex problems with applications in nuclear physics, high-energy physics, and chemical and materials science.

A recently funded LDRD-Exploratory Research project led by Michael Martin (MPA-Quantum, MPA-Q) aims to build a new type of NISQ hardware made from a novel source—individually trapped alkaline earth atoms. This system will comprise several nuclear-spin qubits in strontium. Strontium and other alkaline earth atoms exhibit qualitatively different physical properties, offering performance enhancements over approaches that employ alkali atoms. For example, alkaline earth atoms are readily laser-cooled to temperatures below one micro-Kelvin. They have a precise metastable clock state. They can decouple electronic and motional degrees of freedom when trapped. And their ground state has nuclear-spin degrees of freedom that are protected from decoherence.

The work will establish alkaline earth atoms as a resource for quantum information science—one that has the potential to be competitive with other approaches—and provide a new testbed.
PHYSICAL SCIENCES VISTAS

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for rudimentary quantum algorithms. “Developing quantum hardware and algorithms, in turn, will pave the way for using quantum computers to understand fundamental chemistry and materials science because quantum computation enables simulations of the quantum phenomena that underpin, for example, energy levels of molecules,” Martin said. It also has the potential to produce innovative quantum hardware, identified as a priority by numerous government agencies, including the DOE Office of Science.

The project leverages established hardware and expertise in MPA-Q’s Quantum Technologies team. Principal Investigator Martin researched strontium for his PhD thesis on quantum metrology and many-body physics at the University of Colorado. There, he and co-workers used this alkaline earth species to develop the most precise atomic clock—an exactness that directly benefits other applications, such as quantum information. Co-investigator Leonardo de Melo is a recent addition to the Lab as a postdoctoral research associate and brings expertise in ultracold atom research to the project. Co-investigator Malcolm Boshier has led work in quantum gases at LANL and is the principal investigator of other LDRD-funded work (20180045DR) that has built the capability to trap and cool strontium for atom interferometry. This new LDRD work will build on this infrastructure to trap single strontium atoms in optical tweezers and excite them to strongly interacting Rydberg states. The project also includes a theory collaboration with Ivan Deutsch, a world leader in quantum information science with neutral atoms, at the University of New Mexico. LDRD is internal Laboratory funding for high-risk, high-reward work with the potential to benefit the missions of the DOE and to help position the Laboratory to anticipate and prepare for emerging national security challenges.

MISSION CONNECTION

The work supports the Laboratory’s National Security mission, its Materials for the Future and Information Science and Technology science pillars, and the Laboratory Agenda goal of leadership in the national quantum initiative.

At the Laboratory for Ultrafast Materials and Optical Science, Abul Azad strives to unlock the potential of quasi-two-dimensional metamaterials. These materials, made of subwavelength-resonating structures, are designed to have electromagnetic properties not found in nature. By deciphering and devising the artificial materials, he is contributing to solving the country’s emerging challenges in renewable energy, communications, and sensing.

“Although metasurfaces enable many ultra-thin compact optical devices by enabling unprecedented light-matter interacting, the true potential of metasurfaces is yet to be unlocked,” Azad said. “The space-time duality in Maxwell’s equations suggests further enhancement of metasurfaces’ functionalities by employing additional spatio-temporal modulations.”

For his distinguished service in the advancement of optics and photonics, The Optical Society recognized Azad as a 2020 Fellow. He was cited for his “original and pioneering contributions to the research and development of terahertz metamaterials, few-layer metasurfaces, active metamaterials, and terahertz plasmonics in subwavelength hole-arrays.”

Before joining the Lab in 2007, Azad, who earned his PhD in electrical and computer engineering from Oklahoma State University, was a postdoctoral researcher at Rensselaer Polytechnic Institute and an R&D scientist at Zomega Terahertz Corporation in New York.

He is the recipient of several Laboratory Outstanding Achievement Awards, has served on national and international conference organizing committees, and contributed his expertise to evaluating National Science Foundation and DOE Basic Energy Sciences proposals.
Propelling Los Alamos to the forefront of next-generation accelerator design

Los Alamos National Laboratory is poised to assume a leadership role in the emerging field of high-power radio-frequency (RF) accelerator research thanks to the commissioning of a high-power C-band test facility underway at the Los Alamos Neutron Science Center (LANSCE).

Particle accelerators are established tools for national security and basic science missions. Modern day applications such as x-ray sources—supporting national security, basic science, medical, and industrial needs—require accelerator facilities optimized for cost of construction and operation and for their overall performance.

Internal studies focused on parameters suitable to meet LANL mission needs have concluded that high-gradient acceleration systems at C-band frequencies (4–8 GHz) best meet these conditions. Among technologies used in traditional electron-beam accelerator systems, X-band technology (8–12 GHz) can achieve very high gradient but can lead to severe beam performance limitations, while S-band technology (2–4 GHz) has excellent beam performance but is limited in high-gradient operation. In comparison, C-band accelerators meet efficiency standards, provide the desired high gradients, and simultaneously exhibit excellent beam performance. For instance, compact systems using this technology can provide unprecedented capabilities in an arrangement no larger than a school bus.

The new 50-MW peak power C-band RF test facility will be used for evaluating novel high-gradient accelerator structures with operating gradients in excess of 100 MV/meter—orders of magnitude greater than that of the existing LANSCE linac. Leveraging the Lab's capabilities in materials science, accelerator design and RF technology, and advanced manufacturing, researchers aim to develop high-gradient, high-efficiency RF structures for both compact and facility-size accelerator systems. For example, the new C-band accelerating structures can enable compact, high-gradient electron accelerators such as what might be used to drive a free-electron laser or the ability to reach higher proton energies for use in applications such as proton radiography.

MISSION CONNECTION
The work supports the Laboratory’s National Security and Basic Science missions and the Nuclear and Particle Futures science pillar, particularly its accelerator science and technology thrust by developing accelerator technology capable of unprecedented operation levels, in both accelerating field gradient and efficiency. Improved, custom-designed materials for RF structures are expected to reduce undesired breakdown effects and the introduction of active cooling with cryogens will enable pulsed operation with pulse lengths normally only accessible with much more complex superconducting technology. The new, high-power C-band test facility is playing a crucial role in this LDRD endeavor. It provides a permanent continued on bottom of next page

GET THE DETAILS
Participants: Contributing are staff in Theoretical (T), Accelerator Operations and Technology (AOT), Engineering Technology and Design (E), and Sigma (Sigma) divisions and collaborators from the University of California, Los Angeles and SLAC National Accelerator Laboratory. Funding: Work is funded through the FY20 Laboratory Directed Research and Development (LDRD)-Directed Research project “High-gradient, high-efficiency RF structures: Smart design based on informed break-down suppression” (PI Frank Krawczyk, Accelerator and Electrodynamics, AOT-AE). The C-band test stand is the result of a Science, Technology, and Engineering (DDSTE) strategic investment. Led by Mark Kirshner (RF Engineering, AOT-RFE), the installation was a close collaboration between AOT and LANSCE Facility Operations (LANSCE-FO). Initial materials modeling studies performed in 2018 to assess project feasibility were funded by the LDRD program. Technical contacts: Mark Kirshner (RT test stand), Frank Krawczyk (C-band technology efforts)
Innovative fusion experiment moves toward completion

Researchers running the Plasma Liner Experiment (PLX) at Los Alamos National Laboratory have achieved milestones in an effort to create and form spherically imploding supersonic plasma liners—with the ultimate goal of creating a transformative new compression driver for nuclear fusion energy concepts. The experiments are still at an early stage of development and far from reactor-relevant conditions, but will investigate the promise and feasibility of the proposed innovative architecture for controlled nuclear fusion energy. If successful, the results could ultimately enable terrestrial fusion reactors to be built at substantially lower capital and operating costs than current development trajectories suggest.

For decades, researchers around the world have sought to develop a source of fusion power, as it holds the promise of an almost limitless source of energy. In a nuclear fusion source, power is generated by the heat of fusing atomic nuclei at extremely high pressures and temperatures to the point at which they become a plasma. As an example of nuclear fusion, look to the sun and stars. However, creating such energy in a laboratory environment has proven challenging due to the extreme temperatures and densities required.

LANL scientists at the PLX have studied the merging and shock heating of discrete supersonic plasma jets formed by coaxial plasma guns. They have observed transitions between smoothly interpenetrating regimes and shock-forming regimes depending on the jet densities and relative velocities. These physics clarify options for developing effective plasma liners, which are a potential compressive driver for an approach known as magnetized target fusion (MTF) for achieving fusion energy. In this approach, a heavy hypersonic shell of material, or “liner,” compresses a magnetized fusion fuel target, with the goal of attaining thermonuclear conditions. Other forms of MTF, such as MagLIF at Sandia National Laboratories, start with solid liners. If high-speed, high-momentum, supersonic plasma liners can be developed with sufficient uniformity and timing accuracy, they would be an attractive replacement for solid liners under rep-rate conditions because they are line-replaceable and do not require the repetitive destruction of precision-machined assemblies. Plasma Physics (P-24) staff have conducted detailed experiments with up to 7 plasma guns, and PLX has been upgraded with 18 improved plasma guns installed in a hemispherical configuration. Another 18 are being fabricated and tested at HyperJet Fusion Corporation in Virginia. Ultimately, experiments with a full spherical array of 36 guns will be conducted. Compression of a hydrogen target plasma by the array of plasma jets is proposed in future work.

MISSION CONNECTION

The work supports the Lab’s Stockpile Stewardship and Energy Security mission areas and its Nuclear and Particle Futures science pillar.

GET THE DETAILS

Researchers: Scott Hsu (Physics Division, P-DO); Samuel Langendorf, Kevin Yates, Tom Byvank, John Dunn (all Plasma Physics, P-24); Franklin D. Witherspoon, Andrew Case, Edward Cruz, Sam Brockington, Marco Luna (Hyperjet Fusion Corporation); Mark Gilmore (University of New Mexico); Jason Cassibry, Kevin Schillo (University of Alabama at Huntsville); Roman Sanulyak (Brookhaven National Laboratory); Wen Shih (Stony Brook University); Peter Stoltz, Kris Beckwith (Tech-X Corporation). Funding: DOE ARPA-E ALPHA Program (LANL Program Manager Melissa Fox).


Technical contact: Samuel Langendorf
Realizing damage-resistant materials by controlling microstructural instabilities

While the microstructural strength and plastic response of metals is well studied, the mechanisms leading to metals failure receive disproportionately less attention. High strength, high ductility—that is, maximum deformation prior to failure—and thermal stability are necessary properties for structural materials, especially those encountering extreme environments. Lacking a comprehensive failure model of metals that accounts for these properties, engineers compensate by building in “safety factors” to control for uncertainty in material lifetime. The result is often heavier-than-necessary components in energy applications, such as nuclear reactors and automobiles.

Through “Control of microstructural instabilities in composites (COMIC): A pathway to realizing damage-resistant metals,” an FY20 LDRD-Directed Research project, Los Alamos scientists will provide an understanding of the link between microstructure and failure mechanisms and ductility.

The researchers will use nano-metallic laminates—thin sheets of metal with a microstructure that can be controlled—to single out distinct failure modes common to all metals. Using a combination of experimental, theory, modeling, and simulation approaches, the team will develop an integrated multiscale modeling framework illuminating how a material’s processing affects its properties and ultimately its performance.

This co-design approach leverages the Sigma Complex’s manufacturing science capabilities, the Center for Integrated Nanotechnologies’ characterization capabilities, and the Lab’s high-performance computing capabilities. The project will leverage advanced modeling tools, such as EVP-FFT (elastic viscoplastic fast Fourier transform) and GD3 (generalized discrete defect dynamics), to predict the relation between the onset of failure, loading conditions, and the material microstructure.

In the long term, beyond nanolaminates, COMIC will pave the way toward modeling and designing more-resilient metals processed through conventional or advanced manufacturing techniques.

Images of material failure show three different failure modes that can be triggered in the same material system, which is why nano-metallic laminate composites are an ideal system to understand loss of resilience. Top left: Kink banding. Top right: Necking/void formation. Left: Shear banding.

Mechanical response of Cu/Nb subjected to uniaxial tension (T) or compression (C) along the rolling (RD), normal (ND), or transverse directions (TD).

GET THE DETAILS

Researchers: Laurent Capolungo (principal investigator, Materials Science in Radiation and Dynamics Extremes, MST-8); John Carpenter (co-principal investigator, Finishing Manufacturing Science, Sigma-2); Ricardo Lebensohn (Fluid Dynamics and Solid Mechanics, T-3); Saryu Fensin, Rodney McCabe, Xiang-Yang Liu, and Arul Mariyappan (MST-8); Nan Li (Center For Integrated Nanotechnologies, MPA-CINT); Abigail Hunter (Materials and Physical Data, XCP-5). Reference: “Control of microstructural instabilities in composites (COMIC): A pathway to realizing damage-resistant metals,” Los Alamos Laboratory Directed Research and Development number 20200182DR (2019). Technical contact: Laurent Capolungo

MISSION CONNECTION

The work supports the Laboratory’s Stockpile Stewardship and Energy Security mission areas and Materials for the Future and Information Science and Technology science pillars by advancing efforts to predict material lifetimes under both ambient and extreme radiation and mechanical environments. The modeling capability derived from this work supports the Lab’s efforts at understanding mesoscale evolution in extreme environments and complements national programs and initiatives aimed at testing existing and new materials for use in nuclear reactors.
Single-atom coating enhances efficiency of photocathodes
Application shows promise for accelerator technology improvements

Los Alamos researchers and collaborators have developed a two-dimensional film that not only shields materials under ambient and extreme environments but also enhances some materials properties. The atom-thin coating, dubbed "Atomic Armor," received a 2019 R&D 100 Award and a Gold Medal in the R&D 100 Market Disruptor-Products Special Recognition category. The team’s research demonstrating that the technology can increase the quantum efficiency of photocathodes was featured on the cover of *Physica Status Solidi A* (pictured at right).

DOE has identified the development of new and improved electron sources as one of the highest accelerator R&D priorities for the next decade. To meet DOE’s need for a next-generation electron beam and to advance the scientific frontier of accelerator research, Los Alamos has proposed an x-ray free-electron laser facility—Matter-Radiation Interactions in Extremes (MaRIE). This facility will provide high-energy photons on a variable time scale—from picoseconds to milliseconds—that are required for DOE’s Dynamic Mesoscale Materials Science Capability (DMMSC). This will complement other DMMSC probes, such as proton radiography. Electron beams are generated using photocathodes. Improving the efficiency by which photocathodes generate electrons is a critical step toward achieving next-generation electron beams.

The Atomic Armor team studied the material’s effects on photocathodes relevant to accelerator technology. By coating substrates for antimonide photocathodes with Atomic Armor, they found that as photocathodes were exposed to light at different wavelengths, their quantum efficiency in generating electrons improved by 10%, 36%, and even 80%. Their results provide a pathway toward a simple method of enhancing quantum efficiency in semiconductor photocathodes. The work leveraged LANL’s expertise in materials science, manufacturing, and accelerator technology and its networks of collaborators in the United States and abroad. Specifically, under an LDRD-Directed Research project in 2014, LANL initiated building expertise around interfacing high-quantum-efficiency semiconductor photocathodes with atomically thin crystal layers. LANL is currently the only institution with the expertise.

**MISSION CONNECTION**

The work supports the Laboratory’s Energy Security mission area and its Materials for the Future science pillar. It directly addresses the Lab Agenda initiative to advance accelerator science, engineering, and technology and will enable a solution to DOE’s DMMSC.

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**GET THE DETAILS**

**Researchers:** Hisato Yamaguchi (Finishing Manufacturing Science, Sigma-2); Fangze Liu (Physical Chemistry and Applied Spectroscopy, C-PCS); Jeffrey DeFazio (Photonis Defense); Mengjia Gaowei, John Sinsheimer (Brookhaven National Laboratory); Lei Guo (Nagoya University); Anna Alexander, John Smedley, Nathan A. Moody, Vitaly Pavlenko (Accelerators and Electrodynamics, AOT-AE); Seong In Yoon, Chohee Hyun, Hyeon Suk Shin (Ulsan National Institute of Science and Technology); Matthew Critchley, Daniel Finkenstadt (US Naval Academy); Derek Strom (Max Planck Institute for Physics); Kevin L. Jensen (Naval Research Laboratory); Masahiro Yamamoto (High Energy Accelerator Research Organization). **Funding:** DOE Office of Science US-Japan Science and Technology Cooperation Program in High Energy Physics. **Reference:** “Quantum efficiency enhancement of bialkali photocathodes by an atomically thin layer on substrates,” *Phys. Status Solidi A* 1900501 (2019). **Technical contact:** Hisato Yamaguchi
Form follows function to create a safe, productive, efficient workspace

The Laboratory 5S + Safety initiative is a straightforward approach for creating order in the workplace. Its goal is to eliminate various forms of process waste. These can include wasted motion, wasted time locating materials, wasted supplies, or wasted workplace space.

The 5S in 5S + Safety stands for “sort, set in order, shine, standardize, and sustain.” In each of these steps, the primary focus is always safety. This includes safety for employees who work in a particular area and safety for others who may enter into the area.

“The most exciting part is that when you look at your space from a waste perspective—time, energy, stress—you think about ways to make it easier on your mind and body,” said Christie Davis (Sigma Division, Sigma-DO). “You start preparing your work accordingly.”

Davis and Jacki Mang (LANSCE Facility Operations, LANSCE-FO) are ALDPS champions for the 5S + Safety effort. Under their leadership, areas in the Sigma Complex, the Los Alamos Neutron Science Center, the National High Magnetic Field Laboratory-Pulsed Field Facility, and the Materials Science Laboratory have been treated to the first three steps of the five-step process.

One of the biggest challenges when starting a 5S project, Mang said, is that workers often feel they don’t have the time to organize. However, a successful 5S project should make everyday tasks more efficient. Another benefit is improved continuity of work, even as key personnel retire. A well-labeled workspace allows people to come in and quickly understand which tools are available and what work needs to be done. “It’s empowering,” said Mang. “You don’t have to second-guess if a part is in working order or search for the person who might know.”

The last two steps—standardize and sustain—are critical for success. “So many times, we clean up, but entropy prevails and eventually leaves the space a mess again,” Mang said. “But the 5S program isn’t just about organizing—it’s so much more. It’s about changing your attitude and the workplace culture to make your work life easier, less stressful, and more productive, all of which ultimately make you happier.” Mang and Davis described the 5S+ Safety method as contagious. Once people see or work in a space that’s intuitively organized, they want to spread the practice on their own.

To learn more about the 5S + Safety initiative and ALDPS efforts to improve workspace efficiency, please see int.lanl.gov/org/ddste/aldps/5s-safety.

5S + Safety
Sort: Decide what is needed and eliminate the unneeded items.
Set in order: Arrange and identify necessary items for ease of use.
Shine: Clean the workplace and keep it clean.
Standardize: Create consistency by identifying and applying standards.
Sustain: Maintain the 5S + Safety and establish ways to preserve the work area.
The number of Science Education Community Service hours ALDPS staff served in 2019

The breakdown by activity

- Expanding Your Horizons, 19%
- Science Workshops, 18%
- LANL Summer Physics Camp for Young Women, 17%
- STEM Mentoring, 14.5%
- Los Alamos Employee Scholarship Fund, 11%
- LANL Student Symposium, 10%
- Science Fairs, 6%
- Hour of Code, 2.5%
- San Ildefonso STEM Day, 2%

Science Education Community Service Time is paid time granted to Laboratory full-time and part-time employees at the discretion of their management to assist with science, technology, engineering, and math-related activities. This service helps sustain and strengthen community partnerships that connect the Lab with its Northern New Mexico neighbors.
Copper and steel machine turnings left over from the extensive manufacturing operations in the Sigma Complex.