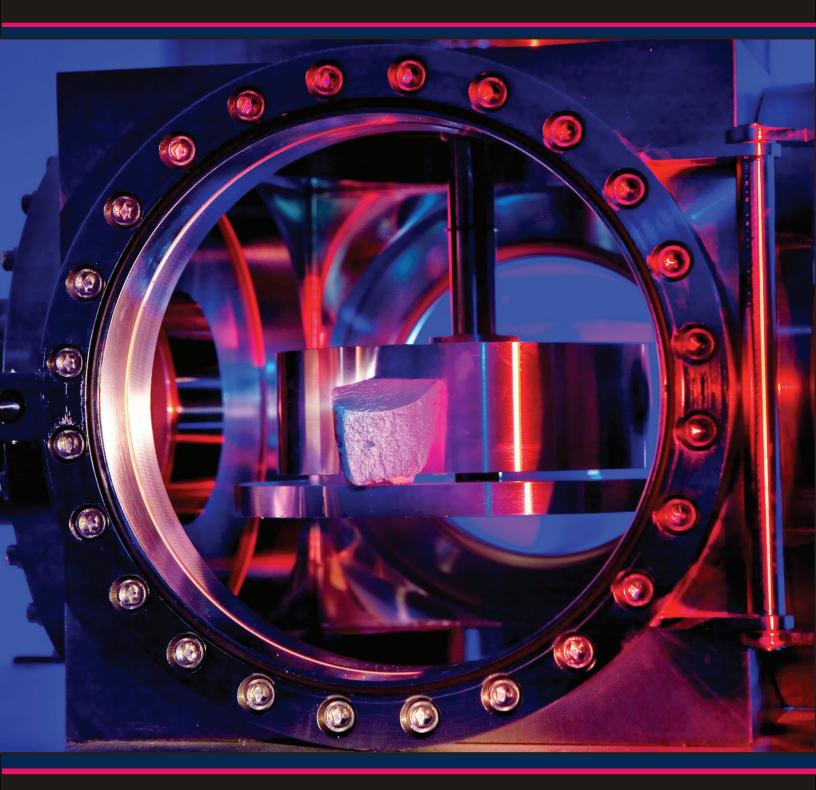
Los Alamos National Laboratory Laboratory Directed Research and Development Program FY23 Annual Progress Report









2023 marks 80 years of science, innovations, and discovery at Los Alamos National Laboratory.











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LA-UR-24-22509



Structure of this Report

The Laboratory Directed Research and Development (LDRD) Annual Report for fiscal year 2023 (FY23) provides a description of the LDRD program at Los Alamos National Laboratory (LANL), including the program's structure and objectives; a summary of the program's value; and highlights of outstanding program accomplishments.

The Annual Report is available at: https://www.lanl.gov/projects/ldrd-tri-lab/annual-reports.php.

On the Cover Cover Image: Photo of ChemCam Laser Chamber, Photo Credit: LANL

On the Inside Cover Historic photo of the Los Alamos Main Gate and the Los Alamos National Security Sciences Building. Photo credit: LANL





Leadership Perspectives

As Los Alamos National Laboratory (LANL) celebrated its 80th 'birthday' in 2023, I couldn't help but reflect on the fact that the Laboratory Directed Research and Development (LDRD) program has been supporting innovate science, research, and development here at LANL for more than a third of that time. Since its inception over 30 years ago, the LDRD program has grown considerably. In 1999, LDRD funded 214 research projects with a budget of \$71M. In fiscal year 2023 (FY23), the LDRD program ended the year funding 490 projects with an overall budget expenditure of \$205M.

Growth is inspiring, energizing, and challenging. As the LDRD program continues to grow, we work closely with leadership and staff across the Laboratory to ensure that the science, research, and development funded through LDRD is truly impactful and strategic. The careful investments made across the year by LDRD play a large role in supporting the Laboratory and our Nation in developing solutions to critical national security issues that include energy security, nuclear security, global security, and environmental security.

LDRD projects are selected for funding through a rigorous and intense peer review process. All projects must align to Laboratory and national security missions. It is the combination of careful alignment and strategic investment that results in the successful outcomes produced by LDRD projects. Projects funded by LDRD have led to prestigious awards, scientific advancements, and have produced influential scientific papers. By tracing scientific achievements that have roots in LDRD, we have been able to determine that close to half of the patents issued to LANL this year are rooted in LDRD work. Additionally, almost half of LANL's FY23 publications have roots in LDRD funded work. The LDRD program is funded with 5-6 percent of the Laboratory's operating budget. These outcomes are confirmation that the LDRD program yields well over its share of scientific advancements and achievements.

This FY23 Annual Report provides an overview of the exciting new research funded by our LDRD program. In this report you will find program highlights, impact stories, and recent accomplishments of LANL's talented research and development staff.





Leadership Perspectives JACOB WALTZ, LDRD DEPUTY PROGRAM DIRECTOR

This year marked the beginning of my second year as the Deputy Program Director for LDRD. I continue to be impressed with the exceptional research and development (R&D) we are able to fund through LDRD.

One of the most valuable aspects of the LDRD program is its role as an outstanding vehicle for attracting promising young scientists and engineers to LANL. In FY23, LDRD supported more than half of the postdoctoral researchers at LANL. Additionally, 367 students worked forty or more hours on LDRD funded projects. The innovative science funded by LDRD attracts students and postdoctoral researchers to LANL, creating an important pipeline of new ideas and talent that contribute to the overall quality of R&D taking place at the Laboratory.

The LDRD program is not unique to LANL. Recognizing the value of collaboration, this year the LDRD programs at Lawrence Livermore, Los Alamos, and Sandia National Laboratories came together to release an Interlaboratory Proposal Call that provided a structured and supported path for interlaboratory collaborations on shared national strategic goals. The planning and release of the call took place in FY23, with project selection taking place in FY24. The response to this new multi-lab call was overwhelming; 79 collaborative proposals were submitted, and requests have already come in from other Labs to participate in future calls.

The LDRD program is a critical venue that allows Laboratory scientists and engineers to pursue cutting-edge R&D in support of national interest and mission development. With our eye continually on the future, the FY23 Annual Report will share with you the projects we fund today that are actively developing revolutionary solutions to tomorrow's challenges.



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Program Description

LDRD DIRECTIVES, OBJECTIVES, AND STRATEGIC CHALLENGES

Laboratory Directed Research and Development (LDRD) helps Los Alamos National Laboratory solve national security challenges through excellence in mission-focused science, technology, and engineering. The Department of Energy (DOE) Laboratory and Site-Directed Research and Development programs are among the most impactful sources of research and development for our Nation. The heart of the LDRD program is high-risk, high-reward research that creates innovative technical solutions for some of the Nation's most difficult challenges. The LDRD programs follow strategic guidance derived from the missions of the U.S. Department of Energy, the National Nuclear Security Administration (NNSA), and the Laboratory.

To execute that strategy, the Los Alamos LDRD program creates a free market for ideas, drawing upon the creativity of the Laboratory's best and brightest researchers. The combination of strategic guidance and grassroots competition provides a continual stream of capabilities that position the Laboratory to enable agile responses to national security challenges.

Funded with five to six percent of the Laboratory's operating budget, the LDRD program makes it possible for our scientists and engineers to pursue cutting-edge research and development in support of mission. This in turn helps the Laboratory, and the Nation, maintain its position of scientific and technological leadership.

LDRD objectives guide the overall program and align with DOE Order 413.2C Chg1. The LDRD program has three objectives: Technical Vitality, Mission Agility, and Workforce Development.



The LDRD program responds to four national security challenges identified in the <u>Strategic Framework</u> (and derived from the 2018 Nuclear Posture Review). This report will illustrate the Los Alamos LDRD program's successes in responding to the LDRD objectives and the national security challenges listed below:

- 1. Provide an agile, flexible, and effective nuclear deterrent.
- 2. Protect against all weapons of mass destruction threats.
- 3Deter and defend against threats in multiple domains.
- 4. Strengthen our energy and environmental national security.

CAPABILITY PILLAR INVESTMENT

LDRD supports Laboratory strategy through our alignment with the Laboratory's Capability Pillars. These six Pillars define strategic investment areas at Los Alamos for present and future missions. All LDRD investments are aligned with the Capability Pillars.

Complex Natural and Engineered Systems (CNES):

- Human-Natural System Interactions: Nuclear
- Engineered Systems
- Human-Natural System Interactions: Non-Nuclear

Information Science and Technology (IS&T):

- Computing Platforms
- Computational Science
- Data Science

Weapons Systems (WS):

- Designer Capability and Certification
- Systems Integration
- Manufacturing and Analysis

The Capability Pillars define six key areas of science, technology, and engineering in which the Laboratory must lead in order to meet the national security challenges of today and tomorrow.

Materials for the Future (MAT):

- Defects and Interfaces
- Extreme Environments
- Emergent Phenomena

Science of Signatures (SoS):

- Nuclear Detonation
- Nuclear Processing, Movement, Aging, Weaponization
- Natural and Anthropogenic Phenomena

Nuclear and Particle Futures (NPF):

- Accelerator Science and Technology
- Applied Nuclear Science and Engineering
- High Energy Density Plasmas and Fluids
- Nuclear, Particle, Astrophysics, and Cosmology



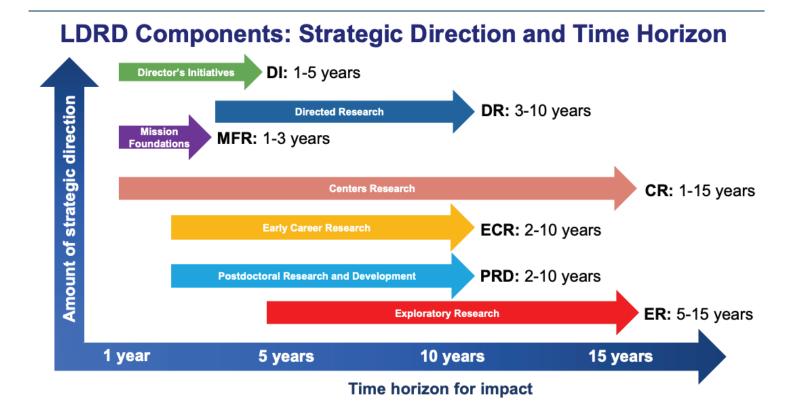
Program Structure OVERVIEW

The Los Alamos LDRD program is organized into seven components with distinct institutional objectives:

- *Directed Research* (DR), flagship investments that create multidisciplinary solutions to complex problems defined by Lab strategy.
- *Exploratory Research* (ER), innovate at the frontiers of technical disciplines.
- *Director's Initiatives* (DI), invest in the Lab Agenda with the rigor and creativity of LDRD.
- *Mission Foundations Research* (MFR), translate discovery into novel mission solutions.
- Early Career Research (ECR), develop next-generation technical leaders.
- *Postdoctoral Research and Development* (PRD), attract and recruit top-quality talent into the Lab's pipeline.
- *Centers Research* (CR), incubate emerging ideas and talent in areas defined by the Lab's Strategic Centers.

The amount of investment in each component is intentionally planned to balance the overall LDRD portfolio in both the time horizon for impact from LDRD projects and the amount of strategic direction from Laboratory leadership that is involved in the selection of projects.

All seven components are discussed in further detail in this report.

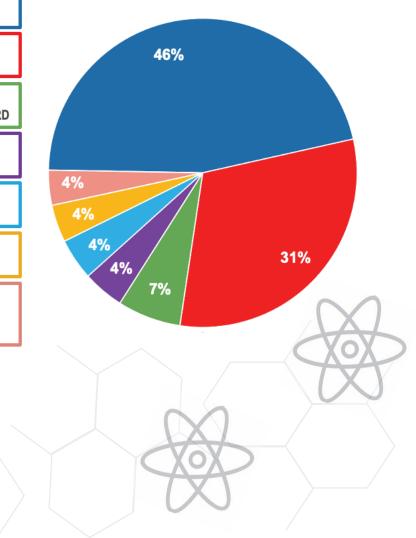


Laboratory Directed Research and Development Program 6



In FY23, the LDRD program allocated \$215M to 490 projects that incurred total costs of \$205M. These projects were selected through rigorous and highly competitive peer review processes and are reviewed formally and informally throughout the fiscal year.

Funds were intentionally distributed across the seven LDRD components. The graphic below illustrates the distribution of funds by showing the total percentage of funds invested in each component area.



Directed Research Create multidisciplinary solutions to complex problems defined by Lab strategy

Exploratory Research Innovate at the frontiers of technical disciplines

Director's Initiatives Invest in the Lab Agenda with the rigor and creativity of LDRD

Mission Foundations Translate discovery into novel mission solutions

Postdoctoral R&D Attract and recruit top-quality talent into the Lab's pipeline

Early Career Research Develop next-generation technical leaders

Centers Research

Incubate emerging ideas and talent in areas defined by the Lab's Strategic Centers

FY23 LDRD Portfolio by Component



DIRECTED RESEARCH: CREATE MULTIDISCIPLINARY SOLUTIONS TO COMPLEX PROBLEMS DEFINED BY LABORATORY STRATEGY

In FY23, LDRD funded 59 Directed Research projects, investing \$94.9M, which represents 46% of the program's research funds.

The Directed Research (DR) component is LDRD's flagship investment. DR projects are aligned to key competency or technology-development areas vital to LDRD's long-term ability to enable the Lab to execute its missions. Funding for individual DR projects is approximately \$2M per year for three years.

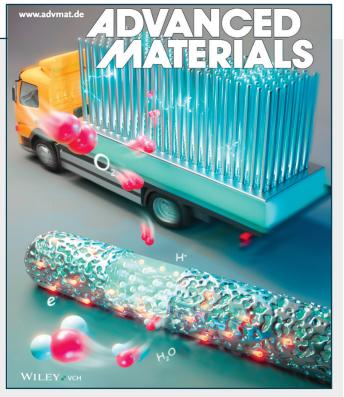
The annual planning for DR directly ties to the Laboratory's Capability Pillars. This planning is communicated through the Strategic Investment Plan (SIP) which is published annually. Laboratory leadership provides strategic guidance to SIP Development Teams associated with each Pillar. The teams then lead a process of engaging with Laboratory staff to identify investment priorities for the upcoming fiscal year that are consistent with and supportive of the long-term Pillar strategy. Priorities may include not just strategic capabilities, but also mission challenges requiring new and innovative approaches.

Directed Research in Action

A promising, more durable fuel cell design could help transform heavy-duty trucking and other clean fuel cell applications. Consisting of nanowires that are less susceptible to corrosion than other designs, the innovative electrode could usher in a new era for fuel cells, which use hydrogen as emission-free power for vehicles.

The project team led by Jacob Spendelow designed and validated a new class of catalyst/electrode architecture, the coaxial nanowire electrode (CANE). Under stress tests the CANE lost only 2% of its performance after 5,000 stress test cycles focused on the support materials, compared to an 87% loss in performance observed with a conventional carbon-based electrode.

With growing interest in the deployment of fuel cells in clean energy applications—particularly in heavy-duty trucking—the CANE architecture holds great promise for enabling a new generation of clean electrochemical energy devices that can replace traditional carbonintensive power generation.



Read more about this exciting new fuel cell design in this Advanced Materials <u>cover article</u>.

Principal Investigator: Jacob Spendelow LDRD project: 20200200DR Structured Electrodes for Energy Conversion, Energy Storage, and Ionic Separations

EXPLORATORY RESEARCH: INNOVATE AT THE FRONTIERS OF TECHNICAL DISCIPLINES

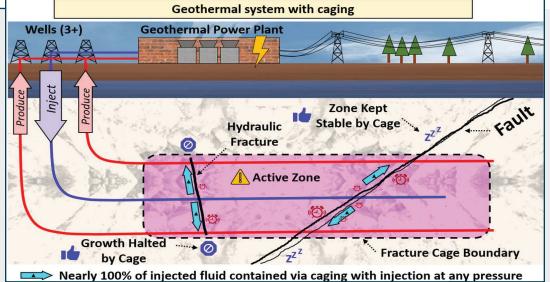
In FY23, LDRD funded 230 Exploratory Research projects, investing \$63.4M which represents 31% of the program's research funds.

The Exploratory Research (ER) component is the most important channel for purely bottom-up creativity at the Laboratory. Initiated by technical staff from across the Laboratory, ER projects explore highly innovative ideas in 10 Technical Categories that underpin Laboratory missions. Funding for individual ER projects is approximately \$350K per year for three years.

Exploratory Research also funds ER Seedlings projects. ER Seedlings projects are funded for 12 months at approximately \$150K per project and are intended to address the most untested, high-risk aspects of a new idea so that, at the end of the project, the now researched and tested idea could then compete successfully for follow-on funding in any venue. The overall objective is to increase acceptance of high-risk proposals that would explore new concepts with the potential to transform the technical field.

Exploratory Research in Action

Several thousand feet below the Earth's surface, rock can reach temperatures that exceed 300 degrees Fahrenheit. Passing fluids through the rock at this temperature harvests enough heat to spin turbines and generate electricity. Enhanced geothermal systems are a promising



technology that could make this energy source available. Smart use of geothermal can dramatically improve air quality while also reducing heating and cooling bills.

Until recently, significant barriers have stood in the way. One particularly concerning problem is induced seismicity, where enhanced geothermal systems could cause tremors in the Earth unless solutions are found to prevent these shakes. At Los Alamos National Laboratory, an Exploratory Research project team led by Luke Frash recently discovered a promising new approach, called fracture caging, to solve this induced seismicity problem.

Experiments, models, and analysis show that fracture caging is both promising and robust. Ultimately, the long-term goal is to enable geothermal to reach its full potential as a widely available, always-on, clean, and carbon-neutral energy source. <u>Read more.</u>

Principal Investigator: Luke Frash LDRD project: 20220175ER Fracture Caging: A new Method to Limit Injection-Induced Seismicity

DIRECTOR'S INITIATIVES: INVEST IN THE LABORATORY AGENDA WITH THE RIGOR AND CREATIVITY OF LDRD

In FY23, LDRD funded 22 Director's Initiative projects, investing \$13.5M which represents 7% of the program's research funds.

LDRD Director's Initiatives (DI) tie directly to critical outcomes within the Laboratory Agenda. The senior Laboratory leaders (typically Associate Laboratory Directors) responsible for the Laboratory Agenda work with the LDRD Program Office and the Deputy Director for Science, Technology, and Engineering to identify strategic growth areas and potential projects. Proposals are held to the same standards of peer review as other LDRD investment components.

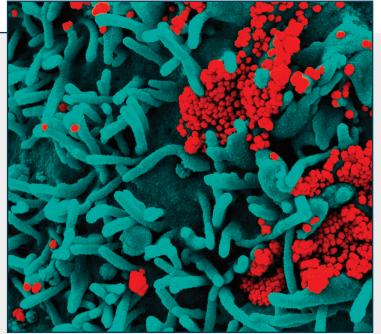
Associate Laboratory Directors (ALDs) typically begin planning before the start of the FY, communicating their project priorities to the LDRD Program Office. The LDRD Office follows with requests for individual proposals and peer review. Most initiatives for the year are in place by January. The duration of Director's Initiatives is between nine months and three years.

Director's Initiatives Research in Action

LDRD researcher Patrick Chain led a DI project focused on developing a system that can track and detect harmful pathogens in the environment, such as wastewater, before they can cause outbreaks that harm human health, handicap our response systems, and damage the economy.

This project was designed to address research and infrastructure gaps by evaluating, adapting, and developing novel methods for making routine surveillance both efficient and effective.

The new capability would allow tracking of known and novel pathogens in relevant environments like wastewater. The project demonstrated that massive improvements in detecting pathogens of interest can be achieved by using already available cuttingedge technologies for enrichments. Similarly, through development of molecular technologies to deplete noise before sequencing, wastewater or any other environmental sample can be used for surveillance.



Colorized scanning electron micrograph of a cell (teal) infected with SARS-CoV-2 virus particles (orange), isolated from a patient sample. Image captured at the NIAID Integrated Research Facility (IRF) in Fort Detrick, Maryland. Credit: Creative Commons CCO and <u>NIAID</u>

Principal Investigator: Patrick Chain LDRD Project: 20230714DI Pathogen Agnostic Detection in Environmental Samples

MISSION FOUNDATIONS RESEARCH: TRANSLATE DISCOVERY INTO NOVEL MISSION SOLUTIONS

In FY23, LDRD funded 28 Mission Foundations Research projects, investing \$8.4M which represents 4% of the program's research funds.

Mission Foundations Research (MFR) is an intentional investment in applied science and engineering relevant to national security missions and addresses mission needs in the technology readiness level (TRL) 3-5 regime. Proposals must respond to "mission problem statements" reflective of mission needs across the Laboratory and are subject to rigorous peer review that assesses alignment with the LDRD program objectives– Technical Vitality, Mission Agility, and Workforce

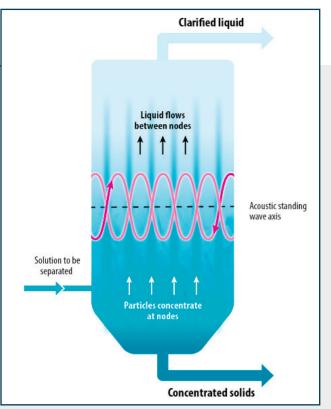
Development. Individual projects are funded at \$215K - \$665K per year, with projects running 1-2 years in length.

Mission Foundations Research in Action

LANL Researchers Jim Coons and Audrey Roman brought together a diverse team of skilled researchers from across the Laboratory to develop a filtration method called UltraSep. Instead of filters, this new technology uses ultrasonic waves and gravity to continuously separate flowing solutions into solid and liquid components. UltraSep operates at a macro-scale, separating flowing suspensions into concentrated solids and clarified liquid components.

The unique filtration method of UltraSep could be a solution to the bottleneck in waste processing that is currently impacting LANL's plutonium facility. In addition to filtering plutonium waste, UltraSep is gaining interest across many other industries that could benefit from this type of filtration, including biofuels, water treatment, and even craft beer.





Solution to be separated enters a vessel from a side channel and flows upward. An acoustic standing wave, oriented perpendicularly to the flow, forces the particles in the solution to concentrate at nodes where they aggregate with other particles. Eventually the aggregates become heavy enough to be pulled to the bottom of the chamber by gravity, meanwhile the liquid, now devoid of particulates, exits out the top of the chamber. Image Credit: Los Alamos National Laboratory

Principal Investigator: Phase 1- Audrey Roman, Phase 2- Jim Coons LDRD Project: 20230467MFR Flocculation and Coagulation of Uranium Hydroxide for Improved Filtration



EARLY CAREER RESEARCH: DEVELOP NEXT-GENERATION TECHNICAL LEADERS

In FY23, LDRD funded 53 Early Career Research projects, investing \$7.9M, which represents 4% of the program's research funds.

The Early Career Research (ECR) component of the LDRD program is designed to strengthen the Laboratory's scientific workforce by providing support to exceptional staff members during their crucial early career years. The intent is to support the development of early career researchers, aiding in the transition from postdoc or student to full-time staff member, and to stimulate research in disciplines supported by the LDRD program. ECR projects are individually funded up to \$240K per year for two years. Early Career Research PIs must have received their highest degree within the last ten years and been hired as a Laboratory technical staff member no more than three years prior to the call.

Early Career Research in Action

Researcher Yu Zhang is leading an ECR project that will develop a quantum many-body theory for polariton chemistry where both matter and light are equally important. Such development will bridge two large subfields, namely quantum chemistry and quantum optics, filling current theoretical and modeling gaps.

Through the work of the project, Zhang is focused on delivering a first-ever ab initio quantum many-body formalism and modeling techniques for polariton chemistry, exceeding any other efforts based on the semiempirical or semi-classical models. Such developments are expected to treat light and matter on equal footing to address the light-matter interaction-induced collective phenomena, filling current theoretical and modeling gaps. The developed techniques will provide a great addition to polariton chemistry, quantum optics, and quantum chemistry research communities.

Zhang recently published a cover article in the journal Physical Chemistry Chemical Physics that is connected to the work of the project. The perspective article summarizes recent theoretical advances in modeling light-matter interactions in chemistry, mainly focusing on plasmon and polariton chemistry. The article explores light-matter interactions, molecular quantum electrodynamics theory, and the challenges of light-matter interactions.



Read Zhang's article, <u>Theory and Modeling</u> of Light-matter Interactions in Chemistry: <u>Current and future.</u>

Principal Investigator: Yu Zhang LDRD Project: 20220527ECR Theory and Modeling of Polariton Chemistry for Quantum Information Science

POSTDOCTORAL RESEARCH AND DEVELOPMENT: ATTRACT AND RECRUIT TOP-QUALITY TALENT INTO THE LAB'S PIPELINE

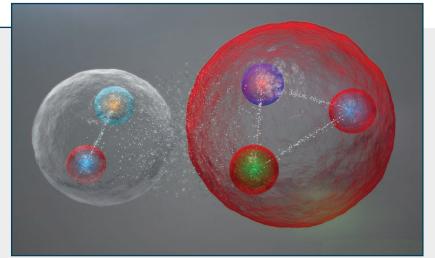
In FY23, LDRD funded 89 Postdoctoral Research and Development projects, investing \$8.8M, which represents 4% of the program's research funds.

The Postdoctoral Research and Development (PRD) component of the LDRD program ensures the vitality of the Laboratory by recruiting early career researchers. Through this component, LDRD funds Postdoctoral Fellows to work under the mentorship of PIs on highly innovative projects. Postdoctoral projects are individually funded up to \$200K per year for 2-3 years. The funding covers the postdoc full time in the first year, then part time in subsequent years to encourage the postdoc to engage with other Laboratory research. The review and selection processes are conducted under the auspices of the Los Alamos National Laboratory Postdoc Program Office.

Postdoctoral Research in Action

This project advances the state-of-the-art of our scientific knowledge and boosts the United States' (US) leadership of the worldwide particle and nuclear physics effort to understand the most fundamental building blocks of the Universe and fundamental forces between them.

Protons and neutrons make up 99% of the visible matter of the universe, including ourselves. They are bound states of quarks and gluons. This project advances methods to study quarkonia- bound states of heavy quarks and antiquarks- to understand the force between them and the structure of protons from whose collisions they are



Bound states of quarks, antiquarks, and gluons, or "hadrons". Image shows initial collision and breaking apart of hadrons, and their recombination into new hadrons. Image Credit: The International Large Hadron Collider at the European Organization for Nuclear Research (CERN)

produced. The project, led by postdoctoral researcher June-Haak Ee and PI Christopher Lee will enhance the scientific output and impact of high-energy particle collider experiments that the US Department of Energy invest heavily in, such as the Relativistic Heavy-Ion Collider and its successor, the Electron-Ion Collider, at Brookhaven National Laboratory.

The goal of this research is to provide the first reliable calculation of double-quarkonium production.

Principal Investigator: Christopher Lee Postdoctoral Researcher: June-Haak Ee LDRD project: 20230857PRD2 New Paradigm for Precision Quarkonium Physics at Future Colliders



CENTERS RESEARCH: INCUBATE EMERGING IDEAS AND TALENT IN AREAS DEFINED BY THE LAB'S STRATEGIC CENTERS

In FY23, LDRD funded 9 Centers Research projects, investing \$7.8M, which represents 4% of the program's research funds.

To infuse new ideas and people into the Laboratory, LDRD has made a commitment to partner with the Lab's "Strategic Centers." The Centers Research (CR) component is focused on developing the Nation's next-generation workforce and leadership talent and serving as an incubator for the introduction of emerging science, technology, and engineering (ST&E) into Laboratory missions. CR projects are typically funded up to three years and single-year per project funding ranges from approximately \$500K-\$1,900K.

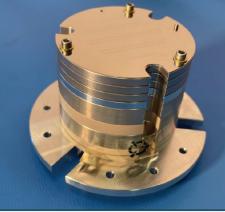
Centers Research in Action

To protect critical United States space assets, we must understand what is orbiting nearby, especially if it is an actively maneuvering spacecraft capable of causing catastrophic harm. Ground-based radar and optical observations have been relied on to detect and monitor orbiting objects, however there is an impending danger that a small and difficult to detect satellite can avoid remote detection and infringe upon an asset's ability to perform nominal operations. The Autonomous Ion Mass Spectrometer Sentry (AIMSS) is a spacebased (in-situ) instrument that will detect thruster plume exhaust or "effluents" of an approaching spacecraft. This will provide an initial alert, like a "canary in the coal mine," to inform satellite operators of potential danger.

The development of AIMSS started as a Center's based project. A prototype was developed. Instrument design and simulation campaigns were conducted. Work on AIMSS will continue through LDRD as a Directed Research project under the leadership of Carlos Maldonado. The

ultimate goal of the continued work is to fly AIMSS on the International Space Station (ISS) and for the first time make mass-resolved measurements of the plume of approaching spacecraft. The project will also leverage and expand unique LANL physics-based modeling capabilities to develop and validate a state-of-the-art model of thruster plume propagation in the space environment as well as its interaction with spacecraft.

Principal Investigator: Carlos Maldonado LDRD Project: 20210528CR Center for Earth and Space Science



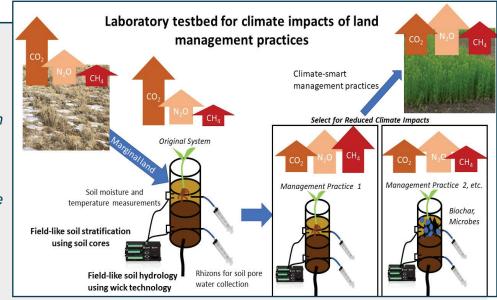


RESERVE FUNDING

Not all of the LDRD budget is allocated to individual projects at the beginning of the fiscal year. The LDRD program employs Reserve funding for strategic initiatives to facilitate institutional agility when addressing time-urgent, national security challenges.

When investing these Reserve funds, LDRD will typically turn to the Associate Laboratory Directors for guidance and priorities. Reserve proposals are held to the same peer review standards as the annual calls.

A total of \$20M in Reserve funds were invested in FY23, with some funds added to existing projects and the remainder used to start 55 new projects during the year. The chart below shows how the funds were invested across the different LDRD components.



with costs easily exceeding \$500 thousand/experiment because laboratory systems do not mimic field conditions accurately enough, leading to increasing consumer costs when climate incentives are applied.

This project led by researcher Sanna Sevanto demonstrated the use of soil cores equipped with glass fiber rope wicks as a laboratory-scale testbed for climate impacts of soil improvements and land use management practices. The project team successfully demonstrated similar carbon (CO2) and nitrous oxide (N2O) emissions from the cores as measured in the field under similar environmental conditions, and the effects of cyanobacterial soil improvement and biocrop cultivation on CO2 and N2O emissions.

The project has led to follow-on funding from the Department of Energy- Fossil Energy and Carbon Management.

Principal Investigator: Sanna Sevanto LDRD Project: 20230616ER Optimization of Arid Systems for Carbon Negative Agriculture and Biomass Carbon Sequestrations and Storage

Reserve Funding in Action

Maximizing carbon sequestration and minimizing greenhouse gas emissions during biomass cultivation for food, biofuel, and biomaterial production is a key component for building cradle-to-grave carbon negative solutions to support climate change mitigation while maintaining food, energy, and natural resource security. Currently, testing climate impacts of land management decisions requires field experiments



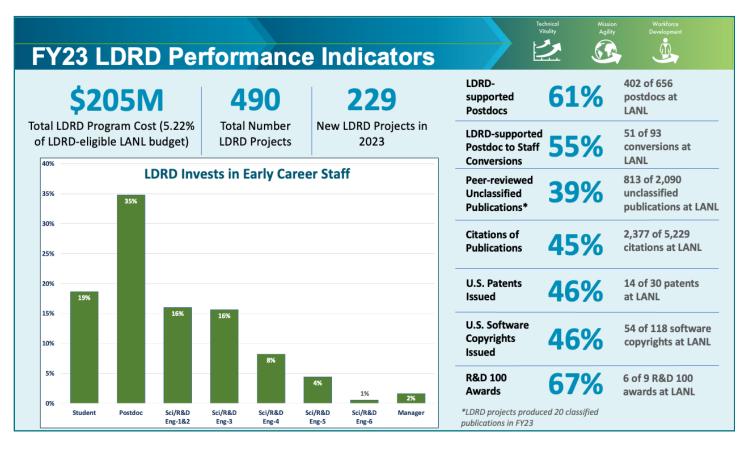
Program Value

Congress established the LDRD program at the DOE National Laboratories in 1991 to foster excellence in science and technology and to ensure the Laboratories are technically vital



and prepared to meet today's needs and tomorrow's challenges. LDRD supports high-risk, potentially high-payoff research and development, serving as a key resource for addressing the science and technology goals of the Laboratory. Through careful investment of LDRD funds, the Laboratory builds its reputation, recruits and retains excellent scientists and engineers, and prepares to meet evolving national needs.

The following metrics show how the LDRD program at Los Alamos successfully addresses the LDRD program objectives of Technical Vitality, Mission Agility, and Workforce Development.



The metrics above show LDRD's impact on key performance indicators and measures. The bar graph, showing total hours charged to LDRD in FY23, illustrates the large engagement of early career staff, postdocs, and students in the LDRD program. As shown in the graph, 19% of the total labor hours charged to LDRD were charged by students, 35% of the total were charged by postdoctoral researchers, and 16% of the total were charged by Scientists/R&D Engineers 1 & 2. It is not uncommon for managers to continue contributing important R&D to a research project, in FY23, 2% of the total time charged was charged by managers working on LDRD projects.

Performance Indicators: LDRD at Los Alamos National Laboratory

This section presents both short and long-term performance indicators that LDRD maintains to evaluate the success of LDRD projects. LDRD yields well over its share of intellectual property, postdoc conversions, publications, patents, and technical awards.

INTELLECTUAL PROPERTY

LDRD funds cutting-edge research that has a large impact on the Laboratory's intellectual property. LDRD projects achieve a disproportionately large percentage of the patents and copyrights issued for Los Alamos research.



US Patents

Number of US patents issued in a given FY.

LDRD supported: Patents issued that would not exist if not for initial work funded by LDRD.

	FY19	FY20	FY21	FY22	FY23
LANL U.S. Patents	53	46	46	38	30
LDRD Supported	20	19	14	19	14
% Due to LDRD	38%	41%	30%	50%	47%

Software Copyrights

Number of software copyrights created in a given FY.

LDRD Supported: Copyrights issued that would not exist if not for initial work funded by LDRD.

	FY19	FY20	FY21	FY22	FY23
LANL Software Copyrights	147	119	120	115	118
LDRD Supported	16	39	48	47	54
% Due to LDRD	11%	33%	40%	41%	46%

Invention Disclosures

Number of declarations and initial records of an invention (a new device, method, or process developed from study and experimentation).

LDRD Supported: Disclosures issued that would not exist if not for initial work funded by LDRD.

	FY19	FY20	FY21	FY22	FY23
LANL Disclosures	118	115	101	73	72
LDRD Supported	39	34	33	30	26
% Due to LDRD	33%	30%	33%	41%	36%

PEER-REVIEWED PUBLICATIONS

The large volume of high-quality scientific contributions produced through LDRD funded work help the Laboratory maintain a strong presence and scientific reputation in the broader scientific community.



Publications

Number of peer-reviewed publications.

LDRD supported: Publications for which LDRD made a substantial contribution.

	FY19	FY20	FY21	FY22	FY23
LANL Publications	2,066	1,971	2,207	1,929	2,090
LDRD Supported	714	678	830	796	813
% Due to LDRD	35%	34%	38%	41%	39%

Citations

Number of times a peer review publication has been cited since the publication year. LDRD Supported: Citations of publications for which LDRD made a substantial contribution.

Publication Year	FY19	FY20	FY21	FY22	FY23
LANL Citations	51,571	68,061	28,574	16,300	5,229
LDRD Supported	23,559	30,519	12,825	6,689	2,377
% Due to LDRD	46%	45%	45%	41%	45%





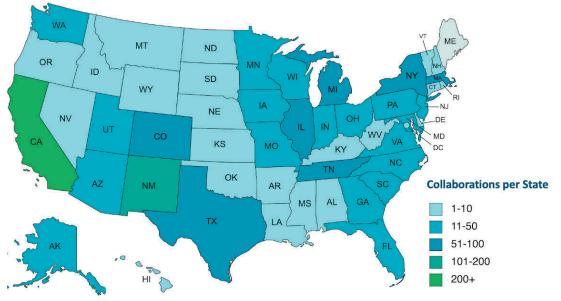
BROAD INTELLECTUAL ENGAGEMENT

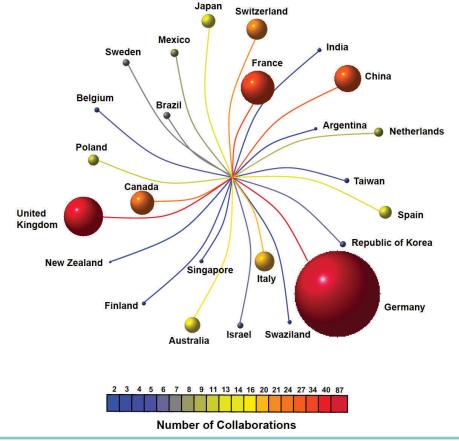
External collaborations are an essential part of the research and development in LDRD. By working with other national laboratories, academia, and industry, LDRD investigators engage with experts across the Nation and around the world. Most external collaborations under LDRD are on a no-exchange-of-funds basis- collaborators use their own funding for the



mutual benefit of working together and promoting scientific/engineering discovery.

In FY22 and FY23 LDRD researchers reported 1,858 external collaborations, including 1,464 collaborations with US scientists and engineers and 394 with foreign collaborators. Collaborations within the United States took place in 49 of 50 states.





The image on the left represents 38 countries in which foreign collaborations with LDRD researchers took place in FY22 and FY23. Circles ranging from smaller to larger indicate the number of collaborations per country, with the range starting at two and going up to 87 collaborations. Not pictured are 13 additional countries in which one collaboration per country took place.

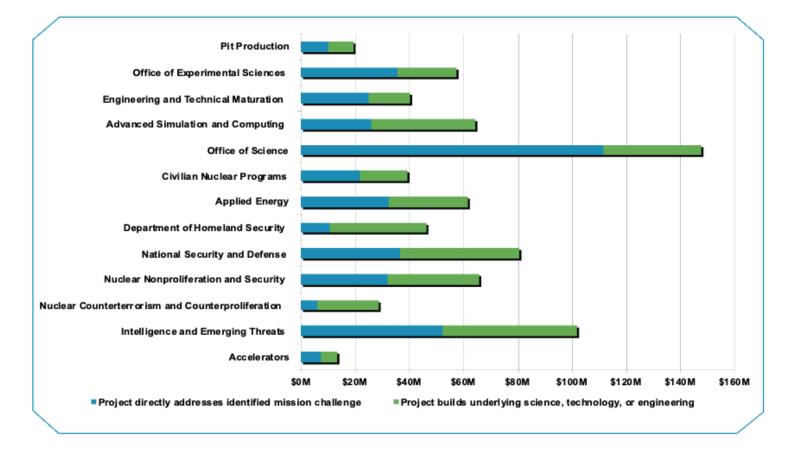


Mission Relevance

Mission relevance is one of the most important criteria in the evaluation of the LDRD program, as well as a potential LDRD project. It is carefully considered in project selection and tracked annually through the data sheet process. Many of the technologies that put Los Alamos on the map have deep roots in LDRD and are valuable to DOE and NNSA mission areas of nuclear security, energy security, environmental remediation, and scientific discovery and innovation.



LDRD work also benefits the national security missions of the Department of Homeland Security, the Department of Defense, and other Federal agencies. As a result, the scientific advances and technology innovations from LDRD provide multiple benefits to all Los Alamos stakeholders, consistent with Congressional intent and the Laboratory's scientific strategy.



Mission Impact of the FY23 LDRD Portfolio (\$M)

Los Alamos LDRD projects are required to address one or more mission areas. Investment in one project often contributes to and impacts multiple missions. The result is that the sum of the total LDRD investment in the relevant mission impact areas shown in the chart above is far greater than the annual LDRD budget.

SCIENCE AND ENGINEERING TALENT PIPELINE

The innovative research and development that LDRD provides is an important vehicle for recruiting the brightest researchers to Los Alamos National Laboratory, where they become innovators and scientific leaders. LDRD is also instrumental in retaining new talent from the student and postdoc pool at the Laboratory.



Postdoctoral Researcher Support

Number of postdoctoral researchers working full- or part-time for the Laboratory. LDRD supported: Postdoctoral researchers charging at least 10% of their time to LDRD.

	FY19	FY20	FY21	FY22	FY23
LANL Postdocs	632	655	665	652	656
LDRD Supported	376	363	391	389	402
% Due to LDRD	59%	55%	59%	60%	61%

Postdoctoral Researcher Conversions

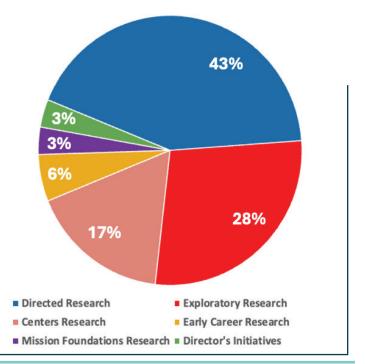
Number of conversions from postdoctoral researcher to a member of the staff. LDRD Supported: Conversion of postdoctoral researchers who charged at least 10% of their time to LDRD in FY23.

	FY19	FY20	FY21	FY22	FY23
LANL Conversions	87	75	81	120	93
LDRD Supported	39	35	44	58	51
% Due to LDRD	45%	47%	54%	48%	55%

Students Supported by LDRD

There are many opportunities for students to play important supporting roles on LDRD projects. For example, a student might work with an early career staff member on a project, where the early career staff member would serve as the PI and the student would serve a significant secondary role to that PI. LDRD is supportive of students working in a Co-Investigator role on any LDRD project.

In FY23, 367 students worked at least 40 hours on LDRD projects. The graph to the right provides a breakdown, by component, of the total student hours charged to LDRD in FY23 for those students who worked 40 or more hours on LDRD projects.





THE LONG-TERM IMPACTS OF LDRD INVESTMENTS

The LDRD program is an investment in the Nation's future, ensuring mission support that is often realized after many years. This section highlights the longer-term (>5 year) impact of LDRD as a national asset. These performance indicators will be updated annually. As it is expected that the data may vary from year to year, long-term running totals will also be included and updated every 5 years.

Background

As part of a commitment to continuous improvement, representatives from each LDRD program at the NNSA Laboratories regularly participate in a working group to share best practices and discuss strategies for tracking the long-term impact of LDRD investments. In FY20, the working group finalized a combination of common quantitative and qualitative long-term indicators, emphasizing a systematic approach. Additionally, the working group recognized that the individual Laboratories may choose to report other long-term indicators that fit their unique missions and capabilities.

Alignment with LDRD Objectives

The collective selection of indicators (both numerical and qualitative) illustrate the long-term payoffs/ success of LDRD, with respect to all three LDRD objectives (Technical Vitality, Mission Agility, Workforce Development). Because indicators crosscut objectives, there is not an intent to provide a 1:1 mapping of indicators with objectives.

Importance of Qualitative Data

The difficulty of developing numerical indicators for success in R&D programs is widely recognized. The metrics working group was able to develop numerical success indicators for both Technical Vitality and Workforce Development. "Success stories" were found to be more flexible to capture the successes in Mission Agility, as well as aspects of the other two LDRD objectives that are not well-captured by numerical metrics.

Tracing impact back to LDRD

Throughout this section, you will see references to "LDRD roots." There is often a lot of discussion with PIs about what it means for an accomplishment to have "LDRD roots." A simple case would be if an idea for an invention arises during an LDRD project and work on the invention is completed during the period of LDRD investment. But R&D often does not advance on such a short timescale. In general, an accomplishment (invention, paper, capability, etc.) is determined to have LDRD roots if there are one or more LDRD projects without which the accomplishment would never have come into being. In other words, if one can identify an LDRD project that was critical to the accomplishment, then it is considered to have "roots" in that LDRD project. Other relevant definitions for the metrics shared are included in the sections to follow.

SCIENCE AND ENGINEERING TALENT PIPELINE

Professional Fellows (American Physical Society)

One relevant indicator of advancement and leadership in an ST&E field is the election of individuals as Fellows of professional societies. This indicator reflects success for both the individual researcher and the Laboratory as a whole. APS Fellowship is awarded based on scientific merit and impact over an extended period of time. (In contrast, some professional

societies may also award Fellow status based on service to the society.) Over the past 10 years, 87% of Los Alamos National Laboratory's (LANL) APS Fellows have had LDRD experience.

	Single-Year Statistics FY21 FY22 FY23			Five T FY14-FY18	Ten Years FY14-FY23	
Total Awards	3	3	1	38	18	56
Awards with LDRD Roots	2	2	1	35	14	49
% with LDRD Roots	67%	67%	100%	92%	78%	88%
Average Years from First LDRD Experience	15	14	10	11.6	12.1	11.8

LDRD and American Physical Society Fellows at Los Alamos National Laboratory



LANL Researcher Elected 2023 APS Fellow has LDRD Experience

Christopher Ticknor was named an APS Fellow for his theoretical and computational advances in the properties of matter under extreme conditions, and for leadership in guiding new research in these fields. Ticknor joined the Laboratory in 2010 as a Director's Fellow and then was one of Advanced Simulation and Computing's first Metropolis Fellows before becoming staff. In 2013, Ticknor became the PI of an LDRD Early Career Research project. During his career, Ticknor has explored a range of physics, including ultracold quantum mechanical scattering, many-body physics of Bose-Einstein condensates, quantum vortex dynamics, dense plasmas and energetic materials.



Тор 2%

The recognition of individuals as esteemed members of technical staff in an ST&E field is an indicator of career advancement. These staff members are named "Fellows" at LANL, Senior Scientists/Engineers at Sandia National Laboratory, and Distinguished Members of the Technical Staff (DMTS) at Lawrence Livermore National Laboratory. The shorthand name used



here, "Top 2%," comes from the intent at each of these Laboratories to limit membership to the top 1% or 2% of scientific and technical staff. The Top 2% awards are comparable to a lifetime achievement award, in this case, for contribution to the Laboratory's mission.

In FY23, all nine of the LANL staff awarded the Fellow recognition had prior experience with LDRD. Fellows typically gain LDRD experience early in their careers, with an average of about 14 years from their first LDRD experience to being named a Fellow.

	Single-Year Statistics			Five	Ten Years	
	FY21	FY22	FY23	FY14-FY18	FY19-FY23	FY14-FY23
Total Awards	4	9	9	22	36	58
Awards with LDRD Roots	3	9	9	19	34	53
% with LDRD Roots	75%	100%	100%	86%	94%	91%
Average Years from First LDRD Experience	10.0	17.1	11.6	13.6	14.0	13.8

LDRD and Top 2% Fellows at Los Alamos National Laboratory

Nine LANL Researchers Elected 2023 Fellows have LDRD Experience



Tariq Aslam, of the Physics and Chemistry of Materials group, began his career at Los Alamos as a graduate student nearly 30 years ago. Since then, he has become a world leader in high-explosives-detonation modeling and algorithm development. In particular, he has been instrumental to detonation shock dynamics modeling. His work has strongly influenced high explosive modeling at Los Alamos, and he has published papers spanning detonation theory and modeling, and computational physics. Aslam's work first began with LDRD in 2022 as a Co-Investigator on a Directed Research project.



Rod Borup, of the Materials Synthesis and Integrated Devices group, is internationally recognized for his scientific excellence and exceptional leadership in the area of fuelcell technologies and is the face of Los Alamos' flagship fuel cell program. He has made significant advances in fuel cell technology for clean energy applications and has an outstanding record of professional service and internal service to the Laboratory. Borup's work first began with LDRD in 2017 as a Co-Investigator on a Directed Research project.

(continued on next page)



expertise in theoretical plasma physics includes kinetic theory and simulation of magnetized plasmas, magnetic reconnection, inertial confinement fusion and weapons physics. Throughout his career, Daughton has made contributions of fundamental importance in all of these topics. Daughton's LDRD work first began in 2008 as a PI on an Exploratory Research project. **Tess Lavezzi Light**, of the Electromagnetic Sciences & Cognitive Space Applications group, has demonstrated nationally recognized leadership in the field of electromagnetic pulse science

William Daughton, of the Primary Physics group, has had an outstanding career spanning multiple topics in both the open science community and the Laboratory's national security mission. His











demonstrated nationally recognized leadership in the field of electromagnetic pulse science as applied to the critical capability of nuclear detonation detection for international treaty monitoring. Through her distinguished career at the Laboratory over the past 24 years, her work has impacted most aspects of the electromagnetic-pulse-sensing program and set the requirements for novel sensor design over the coming decades. Lights' LDRD work first began in 2020 as a Co-Investigator on an Early Career Research project.

Filip Ronning, of the National Security Education Center, is an international authority in condensed matter physics and has made seminal contributions to the understanding of correlated matter. His theory-experiment integration focus was first revealed during his doctoral work at Stanford University, where he pioneered a new understanding of doped Mott insulators. At Los Alamos, his work has mostly revolved around the discovery, understanding and control of quantum phases and phenomena, particularly in f-electron materials. Ronning's LDRD work first began in 2006 as a PI on an Exploratory Research project.

Richard Van de Water, of the Applied and Fundamental Physics group, is an internationally recognized expert in particle physics, with leadership roles in several impactful experiments that have improved the knowledge of the nature of the neutrino and the dark sector. He continues to lead the particle physics community in the development of theory and experimental techniques. His efforts in numerous neutrino experiments have established him as one of the worldwide leaders in particle and neutrino physics. Van de Water's LDRD work first began in 2007 as a Co-Investigator on a Directed Research project.

Hari Viswanathan, of the Energy and Natural Resources Security group, is an international leader in fluid dynamics through fractured systems from the molecular level to field-scale. Viswanathan's pioneering work on fracture simulations made the Laboratory a leader in this field. His research has impacted the energy sector in areas including nuclear waste storage, environmentally friendly fracking fluids, underground CO2 storage, monitoring undocumented orphan wells for methane leakage mitigation, and CO2 sequestration through mineralization. Viswanathan's LDRD work first began in 2006 as a Co-Investigator on an Exploratory Research project.

Ivan Vitev, of the Nuclear and Particle Physics, Astrophysics and Cosmology group, is a world leader on the physics of the quark-gluon plasma and of quantum chromodynamics, the theory of strong interactions. A nuclear theorist at Los Alamos for nearly 20 years, he pioneered novel techniques that drove the field in new directions. He is an international authority in high-energy nuclear physics, recognized for developing the theory of subatomic particle jets in reactions in nuclei, and for establishing methods for strongly coupled plasma tomography. Vitev's LDRD work first began in 2006 as a Co-Investigator on a Directed Research project.

Scott Watson, of the Complex Response Solutions group, is internationally recognized as a leader in all aspects of gas-cavity hydrotesting including sources, detectors, and experimental design. He pioneered the development of multiple-pulse, gas-cavity radiography, which is now a mainstay of the U.S. Stockpile Stewardship Program, allowing the country to certify the stockpile. He has been recognized with numerous prestigious awards including: 10 patents, nine Defense Program Awards, six Distinguished Performance Awards, two R&D-100 awards, two NNSA Gold Awards and the Secretary of Energy Honor Award. Watson's LDRD work first began in 2011 as a Co-Investigator on an Early Career Research project.

American Geophysical Union Fellow



Ruth Skoug, of Los Alamos National Laboratory's Space Science and Applications group, was named an American Geophysical Union (AGU) Fellow in 2023. She was selected for her far-reaching impact to experimental space plasma physics in the solar wind and magnetosphere.

The AGU Fellows program recognizes AGU members who have made exceptional contributions to Earth and space science through a breakthrough, discovery, or innovation in their field. Fellows act as external experts, capable of advising government agencies and other organizations outside the sciences upon request. Since 1962, AGU has elected fewer than 0.1 percent of its members to join this prestigious group of individuals.

Skoug is an expert in solar wind and magnetospheric plasma dynamics and charged particle instrumentation for space physics applications. Her research interests include the development of space plasma instrumentation, solar wind electron distributions, interplanetary coronal mass ejections, solar wind variability and implications for space weather forecasting, global imaging of the magnetosphere and ion composition of the magnetosphere during geomagnetic storms.

Her current scientific activities involve the analysis of solar wind electron and ion plasma data from instruments flying on spacecraft across the solar system, often sensors that she built, calibrated, operates, and for which she leads the science analysis team. She has received NASA Group Achievement Awards for contributions to numerous NASA missions. Skoug is currently the principal investigator for the Solar Wind Electron Instrument on NASA's Interstellar Mapping and Acceleration Probe mission. Skoug's LDRD work first began in 2008 as a Co-PI on an Exploratory Research project.





Workforce



R&D 100 Awards

A relevant indicator of advancement and leadership in an ST&E field is the R&D 100 Award. The prestigious "Oscars of Invention" honor the latest and best innovations and identify the top technology products of the past year. The LDRD Program Offices at each site often partner with sister organizations, such as the Intellectual Property Office and Public Affairs,



to track whether R&D 100 winners (whether in the standard category or special awards) have "LDRD roots." Because of the long development time from idea to practical implementation, the staff on an R&D 100 Award may not be the same staff who worked on the original R&D. Each site's LDRD Program Office engages in an extensive interview process to uncover the details of how the LDRD work led to the celebrated invention.

In FY23, five of the nine R&D 100 Awards received by LANL have roots in LDRD. While there is sometimes minor fluctuation from year to year, multi-year analyses consistently reflect a majority of R&D 100 winners with prior LDRD experience. At LANL, 41 of the 67 R&D 100 awards given to LANL since FY14 have roots in LDRD.

	Single-Year Statistics			Five	Ten Years	
	FY21	FY22	FY23	FY14-FY18	FY19-FY23	FY14-FY23
Total Awards	7	9	9	25	42	67
Awards with LDRD Roots	4	6	5	15	26	41
% with LDRD Roots	57%	67%	56%	60%	62%	61%
Average Years from First LDRD Experience	3.0	9.3	4.8			/

LDRD and R&D 100 Awards Earned by Los Alamos National Laboratory

In 2023 Los Alamos led nine R&D 100 winners. Five of the awards have roots in LDRD. The following five awards are those with LDRD roots.





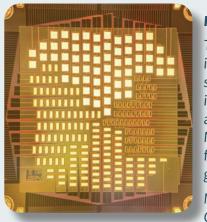
FEVER: Fast Evaluation of Viral Emerging Risks

The current methods of pathogenic viral detection can't keep pace with the high mutation rate of RNA viruses. The FEVER technology of designing diagnostic probes is bolstered against viral mutation. FEVER provides the foundational biosurveillance capability to support global pandemic preparedness and mitigate future outbreaks.

Jessica Kubicek-Sutherland led the Los Alamos team of Brian Foley, Samantha Courtney, Jason Gans, Zachary Stromberg, and James Theiler. The late Karina Yusim initially directed the researchers.



FEVER also received the Gold Medal Special Recognition Award for Corporate Social Responsibility, which honors organizational efforts to be a greater corporate member of society; and the Gold Special Recognition Award for Battling COVID-19, which highlights any innovation that was employed to battle the worldwide COVID-19 pandemic. <u>Watch the video</u>.



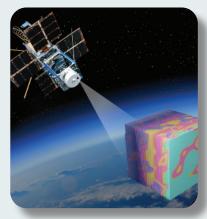
HXI: Hyperspectral X-ray Imaging Detector

This new capability in energy resolution and efficiency for material analysis in scanning electron microscopes allows researchers to measure material signatures at the nanoscale. Such analytical capabilities are especially important for samples that vary in composition on very small length scales, and where macroscopic material properties depend on microscopic features. Nanoscale mapping could benefit the semiconductor fabrication industry, forensics, materials science, environmental science, biological science, and geological science fields.

Mark Croce led the Los Alamos team of Enrique Batista, Eric Bowes, Matthew Carpenter, Christopher Fontes, Joseph Kasper, Katrina Koehler, Daniel McNeel, Michael Rabin, Katherine Schreiber, Benjamin Stein, Emily Teti,

Gregory Wagner, Jacob Ward, Lei Xu, and Ping Yang Partner organizations included the National Institute of Standards and the University of Colorado, Boulder. <u>Watch the video</u>.

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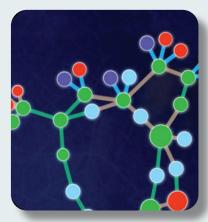


NACHOS: Nano-satellite Atmospheric Chemistry Hyperspectral Observation System

The novel instrument delivers trace gas detection capabilities in a small, lightweight package for space. It analyzes the spectral fingerprint of each toxic gas, processes raw data and supports attribution of harmful gas emission sources on Earth. NACHOS supports space-based, airborne, and ground-based mission deployment, including trace gas detection from CubeSats, deepspace planetary missions, remote monitoring ground stations, and airborne monitoring from drones. Two NACHOS CubeSats have flown in space.

Steven Love led the Los Alamos team of Kerry Boyd, Michael Caffrey, Malakai Coblentz, Magdalena Dale, Nicholas Dallmann, Manvendra Dubey, Bernard Foy,

Tracy Gambill, Arthur Guthrie, Markus Hehlen, Ryan Hemphill, Gregory Lee, Kristina McKeown, Hannah Mohr, Donathan Ortega, Logan Ott, Glen Peterson, Kirk Post, Michael Proicou, Claira Safi, Daniel Seitz, Paul Stein, James Theiler, Christian Ward, and James Wren. <u>Watch the video.</u>

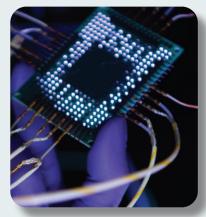


PowerModelsONM: Optimizing Operations of Networked Microgrids for Resilience

Modern society is critically dependent on the electric power grid. This optimization software package models restoration and reconfiguration of electric power distribution feeders featuring networked microgrids. The technology uses real-world data from utilities and has been tested with power hardware-in-the-loop, allowing resilience scenarios to be validated without risk to the real system. Utilities can use PowerModelsONM to plan for networked microgrids to support increased resilience during and rapid recovery after electric grid outages.

Los Alamos led the joint entry with the National Renewable Energy Laboratory,

Sandia National Laboratories, and the National Rural Electric Cooperative Association. Russell Bent directed the Los Alamos team of David Fobes, Arthur Barnes, Jose Tabarez, Harsha Nagarajan, Hassan Hijazi, Smitha Gopinath, Kshitij Girigoudar, Haoxiang Yang, Thabiso Mabote, Matthew Job, and Zhen Fan. <u>Watch the video.</u>



Solution-processed Perovskite Crystalline Films (SPeC)

This technology combines molecular engineering of earth-abundant materials with a thin film coating method that can be adapted to mass production and

scaled for size. Processing costs less and uses much less energy compared with current approaches. The near-single crystal layer films create many fewer crystalgrain boundaries and defects than other semiconductor fabrication methods. Benefits include more efficient solar cells, brighter and fully color-tunable light-emitting diodes (LEDs), and more sensitive X-ray detectors.



Wanyi Nie led the team of Sergei Tretiak, Hsinhan Tsai, and 🛛 🖬

Shreetu Shrestha. SPeC also received a Bronze Special Recognition Medal for Market Disruptor - Products. <u>Watch the video.</u>

Additional LDRD Spotlights



LDRD Researcher Elected to lead the American Physical Society's Topical Group in Plasma Astrophysics

Fan Guo, physicist in the Nuclear and Particle Physics, Astrophysics and Cosmology group at Los Alamos National Laboratory, has been elected to lead the American Physical Society's Topical Group in Plasma Astrophysics (GPAP). The four-year leadership role starts with the position of vice chair, followed by the positions of chair-elect, chair, and pastchair.

Guo became a research scientist in the Laboratory's Theoretical division in 2016, having joined the Lab as a postdoctoral researcher in 2012. Guo's work with LDRD first started in 2015 as a Co-Investigator on an Exploratory Research project.



"It is a great honor to award these two outstanding scientists this year's Global Security Medal," said Nancy Jo Nicholas, associate Laboratory director for Global Security. "The experimental and computational subject matter expertise Juan and Kevin represent as a team enabled transformational contributions to the community. I look forward to many more accomplishments from this dynamic team."

Workforce

Development

LANL researchers Juan Duque, left, and Kevin Mitchell.

Meet the Global Security Medal Winners

Juan Duque and Kevin Mitchell have been awarded the 2023 Los Alamos Global Security Medal. The award recognizes the exceptional achievements of active or recently retired employees who have made significant contributions to the Laboratory's global security mission.

Duque and Mitchell received this year's Global Security Medal for growing the Laboratory's capabilities in remote sensing. This journey began with government agency funding, which was then strengthened through LDRD investment to expand the test site and advance the algorithms through machine learning. The LDRD investment furthered their science through out-of-the-box thinking and ingenuity, gaining large-scale recognition for the program and the Laboratory. One sponsor stated that no other test/calibration site or team in the world provides an equivalent capability and responsivity for U.S. remote sensing needs spanning a wide range of targets.

Duque's LDRD work first began in 2008 as a Postdoc on an LDRD Postdoctoral Research Project, receiving a Postdoctoral Distinguish Performance Award in 2010.

Mitchell's work on synthetic training data supported the LDRD funded work, bringing together a combined effort that grew the Laboratory's remote sensing capability.

LDRD Program Accomplishments TOP SCIENCE IN THE NEWS

First Hints of Nuclear Fission in Cosmos Revealed by Models, Observations

New research suggests fission may operate in the cosmos during the creation of the heavy elements. Combing through data on a variety of elements that reside in very old stars, researchers have found a potential signature of fission, indicating that nature is likely to produce superheavy nuclei beyond the heaviest elements on the periodic table.

"People have thought fission was happening in the cosmos, but to date, no one has been able to prove it," said Matthew Mumpower, a theoretical physicist at Los Alamos National Laboratory and co-author of a paper in <u>Science</u> presenting the research.

Using the latest observations, the researchers found a correlation between light precision metals like silver and rare earth nuclei like europium. When one of these groups of elements goes up, the corresponding elements in the other group also increase — the correlation is positive.

The team tested all the possibilities and fission was the only explanation that was able to reproduce the trend. "This is incredibly profound and is the first evidence of fission operating in the cosmos, confirming a theory we proposed several years ago," Mumpower said. "As we've acquired more observations, the cosmos is saying hey, there's a signature here, and it can only come from fission."

Mumpower developed the fission models used to predict and guide the observational findings, which were led by Ian Roederer of North Carolina State University.

The new analysis found a pattern that provides a clear signature of fission creating these elements and a similar pattern of elements slightly heavier and higher on the periodic table.



Two neutron stars colliding to release neutrons that radioactive nuclei rapidly capture. Image Credit: Los Alamos National Laboratory

"The correlation is very robust in r-process enhanced stars where we have sufficient data. Every time nature produces an atom of silver, it's also producing heavier rare earth nuclei in proportion. The composition of these element groups are in lock step," Mumpower said. "We have shown that only one mechanism can be responsible — fission — and people have been racking their brains about this since the 1950s."

"At Los Alamos, we developed nuclear fission models because we can't measure everything that's relevant for weapons research as part of the Laboratory's mission," Mumpower said. The models allow physicists to interpret experiments and fill in data when measurements are lacking. Since the United States halted testing of nuclear weapons in 1992, experimental data on fission has been limited.

The models perform exceptionally well when compared to measured data and thus give credence to their extrapolations where there are no measurements. The nuclear inputs of both shortlived and long-lived species are required for studies of heavy element formation, Mumpower said. Fission yields are products of the process of splitting relatively heavy atoms into lighter ones — the same process used in nuclear weapons and reactors.

This work was supported by LDRD project 20200384ER. Read the article <u>here</u>.

TOP SCIENCE IN THE NEWS

Supercomputer Simulation Attacks Problem of Drug-resistant Bacteria

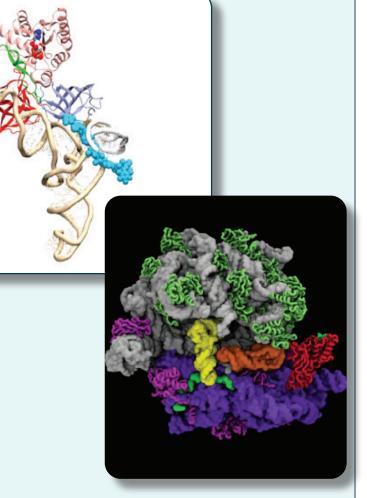
UNDERSTANDING MOLECULAR PROCESSES CAN IMPROVE THE ANTIBIOTICS AND VACCINES THAT FIGHT DISEASE

A first-ever, atom-by-atom supercomputer simulation shows how antibiotics kill bacteria and illustrates other processes of the molecular machinery in living cells. The research opens fresh pathways to improving antibiotics, designing new ones to fight drug-resistant bacteria, and developing vaccines for viruses such as SARS-CoV-2, which causes COVID-19.

"The ribosome is the central informationprocessing molecular machine in all life forms. It has to decipher information about accepting correct amino acids and rejecting incorrect amino acids for building proteins in the cell," said Karissa Sanbonmatsu, a structural biologist at Los Alamos National Laboratory.

"Using the supercomputers at Los Alamos, we're able to image this process atom for atom and show how antibiotics affect that process," Sanbonmatsu said. "Studies like these are critical for combatting the emerging crisis of antibiotic-resistant bacteria."

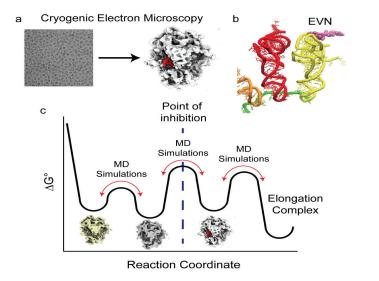
"Antimicrobial resistance is on the rise due to overuse in medicine and agriculture," said Dylan Girodat, first author of the paper, who developed the project with Sanbonmatsu. Now an assistant professor at the University of Arkansas, Girodat was a postdoctoral fellow at Los Alamos when he and Sanbonmatsu performed the research. "To combat antimicrobial resistance, we must understand how conventional antibiotics work if we want to develop novel ones."



In the first image (upper left), a molecular simulation on a supercomputer at Los Alamos National Laboratory reveals how the antibiotic evernimicin (light blue) interacts with transfer RNA molecules (gold) in the ribosome of bacteria, shedding new light on how the antibiotic's chemistry makes it kill bacteria. The second image from a simulation (lower right) shows "incorrect" transfer RNA (orange) moving into a ribosome without antibiotic.

Sanbonmatsu's lab at Los Alamos coordinated the ribosome research, which also has implications for cancer treatments and understanding the origins of life. The research closely integrated singlemolecule experiments led by Scott Blanchard, a dynamic structural biologist at St. Jude Children's Research Hospital, with simulations on a Los Alamos supercomputer by Girodat.

Messenger RNA, or mRNA, carries codes with the information for creating specific proteins in a cell.



Structural dynamics of antibiotic dependent protein synthesis inhibition. (a) Cryogenic electron microscopy, (left) floated carbon grid with ribosomes in complex with mRNA, (right) 6.8 Å resolution structure of a ribosome (white) with mRNA (red). (b) Snap shot of evernimicin (EVN - pink) acting as a steric road block to the movement of the tRNA (yellow) into the ribosome. (c) Cryogenic electron microscopy resolved structures of ribosome complexes along the reaction coordinate of mRNA binding.

The ribosome decodes this genetic information by reading codes from the mRNA, pulling the mRNA through the ribosome similarly to the way a cassette tape player "reads" information off a tape. The ribosome looks up the codes in a molecularinformation table, which is a suite of molecules called transfer RNAs, or tRNA, to select specific amino acids and manufactures proteins based on those encoded instructions.

For each code unit in the mRNA, the ribosome sorts through amino acids and chooses the correct amino acid corresponding to that code unit, while rejecting incorrect amino acids. The tRNA molecules deliver the essential building blocks of proteins to the ribosomes. The ribosome then assembles a protein by adding the correct amino acid.

Many antibiotics work by gumming up this molecular machinery in bacteria's ribosomes, Sanbonmatsu said. The drugs either grind the machine to a halt or cause errors in the information processing, resulting in malformed proteins, killing the bacteria.

In contrast, mRNA-based vaccines target human ribosomes, convincing them to make COVID virus proteins (the spike protein), which helps inoculate the body against the virus. A deeper understanding, attained from supercomputers, of how the ribosome can read mRNA will help researchers design more effective antibiotics and vaccines.

"About 50% of all antibiotics inhibit ribosome function, so we know that this is an effective strategy for antibiotics," Girodat said. "To develop new antibiotics, we need to understand how ribosomes work at an atomic level."

To that end, the research team simulated the molecular dynamics of the interactions between ribosomes and tRNA.

"Our simulations revealed that incorrect tRNA molecules do not adopt the proper geometry when interacting with ribosomes," Girodat said. "By introducing the antibiotics gentamicin, neomycin, evernimicin and hygromycin in these simulations, we demonstrated that antibiotics influence the geometry of tRNA, causing the ribosome to incorporate incorrect tRNA or none at all."

"Ribosomes are massive biomolecules, and achieving the necessary timescales to observe ribosome dynamics requires massive computational resources, such as those available at the highperformance compute cluster at Los Alamos," Girodat said.

The work is funded through LDRD project 20210759PRD1. Read the article <u>here</u>.

TOP SCIENCE IN THE NEWS

Advancing Next Generation Small Reactors

Los Alamos nuclear engineer, Holly Trellue, is leading a project that will help advance the next generation of small, nuclear reactors.

Currently, all commercial nuclear reactors (called light-water or conventional reactors) built in the United States use uranium dioxide as fuel with water as a moderator that helps slow down the neutrons produced by fission. The fission creates heat, and the power plant uses that heat to turn water into steam, which then turns a turbine to produce electricity. The reactor core (where the fissions take place) must be kept cool or the nuclear fuel will overheat and melt. Water is used as a coolant.

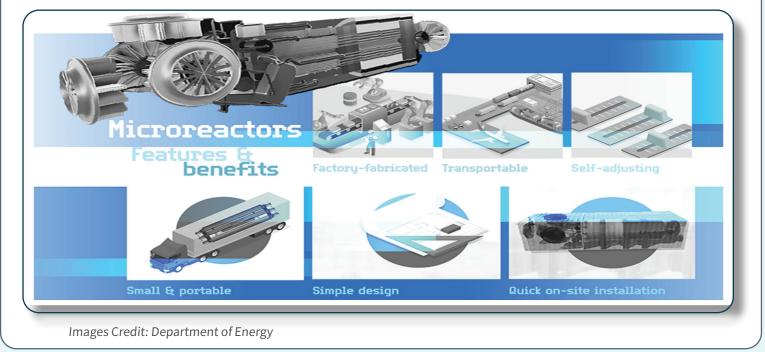
While there are some new reactors located in Georgia that began operation in July of 2023, most reactors are older, with an average age of 42 years. The oldest commercial reactor, located in New York, began operation in December 1969. New reactor development in the United States has been slow due to concerns over size, fuel types, and safety. have increased both the safety and efficiency of nuclear reactors. "We are doing research on highdensity fuels that don't require as much enrichment, which means the reactor can be scaled down," says Josh White, a senior scientist in the Lab's Materials Science and Technology division. "Decreasing the amount of uranium needed in the reactor makes the reactors smaller and easier to build."

One new fuel type under development is high-assay, low-enriched uranium (HALEU), which contains an increased concentration of uranium-235 (the fissile uranium isotope) compared to commercial Light Water Reactors. This new fuel type improves reactor performance, reduces refueling needs, and decreases waste volume. HALEU would allow researchers to design new types of reactors that can operate for decades without refueling and that produce less waste.

So, what will these advanced reactors look like? When it comes to nuclear reactors, bigger isn't necessarily better. Los Alamos scientists are working with industry partners to develop small modular reactors and microreactors—diminutive, easy-toproduce, portable sources of nuclear energy.

However, developments in new fuels and materials

Microreactors can produce between 0.1 and



20 megawatts of energy, whereas the smallest operating U.S. nuclear power plant produces 581 megawatts. To put that in perspective, a microreactor generating 10 megawatts of energy can produce around 10 years or more of electricity for more than 5,000 homes, 24 hours a day, 7 days a week.

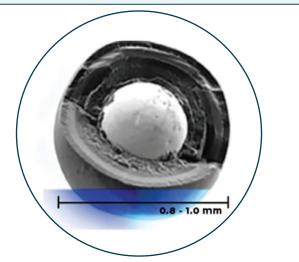
Los Alamos scientists are also working on the development and testing of new materials for moderators and reactor construction. Moderators are any material placed in the reactor core to slow down neutrons and create more fissions. By experimenting with different types of moderators, Lab researchers are finding ways to make reactors safer. "The benefit of solid moderators is if the temperature gets too hot, the reactor will passively shut down without an operator," White says. "Safety is dramatically enhanced without requiring the human part of the equation. It's not possible for the reactors to fail. They are inherently engineered not to fail."

One of the moderators Los Alamos scientists are developing is yttrium hydride—a rare earth metal and hydrogen mixture. "This moderator allows us to make smaller, more efficient microreactors that produce fewer waste products," says Trellue.

Other materials research focuses on methods used for cooling, such as replacing water cooling with molten salt, and advanced materials to meet the unique demands of the smaller reactor designs.

"To be able to produce power efficiently in a microreactor," Trellue explains, "we would like to be able to operate at as high a temperature as possible, so we are experimenting with different structural materials, advanced fabrication methods, and new approaches to shielding."

She points out that one of Los Alamos' key contributions to reactor advancements is the development of heat pipes that use passive cooling to make the reactors safer and more portable.



Tristructural isotropic (TRISO)-coated particle fuel is a key part of many advanced reactor designs. Image Credit: Los Alamos National Laboratory

"Los Alamos is the expert on heat pipe technology," she says. "As a Lab we have always had great ideas, state-of-the-art facilities, and expertise to contribute to advanced reactor systems."

If it seems as though Los Alamos researchers are reaching high with their new reactor ideas, they are—including all the way to outer space. The Lab has supported research on nuclear propulsion technology and the possibility of using reactors to power human outposts on the Earth's moon and Mars. In 2018, the Laboratory—in conjunction with the National Aeronautics and Space Administration and the Department of Energy—tested a system named KRUSTY (short for kilopower reactor using Stirling technology).

Development of new technology and collaborations to support both space and terrestrial applications will continue at the Lab. Trellue says she has many reasons to feel excited about this work, including "developing clean energy sources, helping remote communities meet their energy needs, being part of the nuclear growth of this country, and developing this energy source."

This work was supported by LDRD project 20220084DR. Read the article <u>here</u>.

LDRD IMPACT STORY

Envisioning a Regional Hydrogen Economy

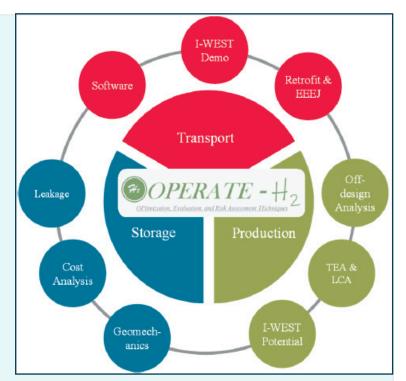
A HOLISTIC APPROACH TO EVALUATING HYDROGEN IN THE INTERMOUNTAIN WEST

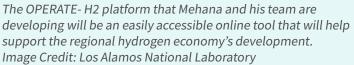
With global energy use increasing, Los Alamos National Laboratory is developing new ideas for reliable, secure, and sustainable carbon-neutral energy solutions for the nation.

Regionally, the United States' Intermountain West is poised for a major energy transition. Arizona, Colorado, Montana, New Mexico, Utah, and Wyoming all have fossil fuel-based economies, and the United States has set the goal of achieving a carbon pollution-free power sector by 2035 and a net zero emission-economy by 2050. The Intermountain West Energy and Sustainability Transitions (I-WEST) initiative is sponsored by U.S. Department of Energy and led by Los Alamos National Laboratory.

The initiative's goal is to better understand how the coming energy transition will affect economies, resources, infrastructure, workforces, and energy justice across the Intermountain West. Among its other focus areas, I-WEST is exploring how hydrogen can help the region reach carbon neutrality in the decades to come. "Hydrogen has the potential to help decarbonize sectors of the economy that are hard to decarbonize by other means" says Mohamed Mehana, a scientist at Los Alamos.

Hydrogen has many advantages as an energy technology. Cars and trucks powered by hydrogen fuel cells produce no tailpipe emissions, and hydrogen yields fewer greenhouse gas emissions than natural gas when burned. It is also possible to produce "clean" hydrogen using water and renewable energy sources, a process that yields very few carbon dioxide or other greenhouse gas emissions.





At present, hydrogen is not a large part of the regional energy mix. For hydrogen to become a major part of the region's energy economy, a range of technologies will need to be deployed concurrently, facilitating the large-scale production, storage, and distribution of hydrogen.

Mehana leads a project that is helping coordinate the development and deployment of varied technologies. The project "Risk-informed Assessment of Hydrogen Storage, Production, and Infrastructure" is funded through LDRD's Mission Foundations Research (MFR) program. MFR supports applied science and engineering relevant to national security missions, with an emphasis on improving the Laboratory's capacity to translate discovery into innovative solutions.

Mehana's project is developing a range of tools. The team of seven scientists, students, and postdocs with wide expertise initially focused on the "storage" side of the hydrogen economy. The team holistically combined tools to evaluate geologic reservoirs, such as salt beds and depleted oil wells, to evaluate reservoirs for hydrogen storage.

According to Mehana, subsurface hydrogen storage is likely to be an important part of the coming hydrogen economy. "Given the scale of production that we will likely need, current surface storage options for hydrogen don't have the capacity to decarbonize the grid," Mehana says. "Subsurface storage has the potential to be more efficient, safe, and secure than current solutions."

The project has already developed OPERATE_H2, a graphical user interface that makes subsurface hydrogen storage models available to non-technical users. OPERATE_H2 leverages a set of machine learning models trained on a comprehensive database of high-fidelity reservoir simulations. This smart, user-friendly platform will allow I-WEST stakeholders to visually explore possible options for hydrogen storage. The science-based tools will empower stakeholders ranging from technology developers and deployers to Sovereign Nations to state-level leaders and economic developers. The project team will further develop its models for geologic hydrogen storage, adding cost analyses and risk assessment modules to the OPERATE_H2 platform, and will evaluate a broader range of hydrogen production technologies.

Thus far, the Risk-Informed Assessment project team has focused its efforts on quantifying hydrogen production through steam methane reforming (SMR), which involves heating natural gas to produce hydrogen. Going forward, the project team will broaden its analysis of SMR while also evaluating production techniques like autothermal reforming, partial oxidation, and water electrolysis. The goal is to develop tools that allow users to evaluate locations for hydrogen production in the Intermountain West.

Hydrogen transportation is a major consideration in the project. The team envisions potential future situations where hydrogen production expands, which could make a pipeline network necessary. The project team can develop tools that



Los Alamos researcher Mohamed Mehana

will help optimize hydrogen transport infrastructure based on the team's experience with Los Alamos' SimCCS software—a 2019 R&D 100 award winner that enables the design of carbon dioxide capture, transport, and storage infrastructure.

The OPERATE_H2 platform will be easily accessible to non-technical experts and help spur the regional hydrogen economy's development. Mehana says that the project team envisions OPERATE_H2 as a platform that will continue to evolve, incorporating research conducted by parties beyond the Laboratory.

The team has given several presentations at I-WEST workshops, most recently by Principal Investigator (PI) Mehana and the Co-PI Bailian Chen, and will lead future scientific collaborations.

"We'll be able to incorporate other groups' models and analyses into OPERATE_H2, to advance the capabilities," Mehana says. "It's a platform for everyone."

This work is funded through LDRD project 20230411MFR. Article written by Jake Bartman, LANL.

LDRD LONG-TERM IMPACT STORY

Connecting the Dots

A LOS ALAMOS DISCOVERY THAT COULD SHAKE UP OPTICAL COMMUNICATIONS, MEDICAL IMAGING, AND THE \$515 BILLION SILICON CHIP INDUSTRY

Recently, Los Alamos postdoc Namyoung Ahn made the latest contribution to a discovery that could someday soon shake up the entire computing industry. Ahn sent electricity coursing through a device he and a team of colleagues had built over the past 20-plus years that could one day turn quantum dots, synthetic nanoparticles about 1/10,000th the thickness of a human hair, into a laser capable of communicating information between microelectronic devices. This time, Ahn saw a tiny spot on the glass wafer glow a brilliant red.

Ahn conducted his research as a postdoc under Victor Klimov, a Los Alamos scientist who started working with quantum dots in the late 1980s and brought his work to Los Alamos in 1995. Klimov wanted to harness the dots' unique quantum properties to make electrically driven lasers that could be fabricated cheaply using simple benchtop chemistry and could sit on any substrate, including silicon. If realized, such devices could send and manipulate information using light alone. The idea could be a boost to microelectronics and the \$515 billion-dollar annual silicon chip industry. Phones, computers, weapons, manufacturing, transportation, communication—silicon chips are the beating heart of very nearly all modern technologies, and the industry is forecast to crest a trillion dollars by decade's end. Electrically driven lasing quantum dots could revolutionize all of it.

Ahn watched a monitor as the line indicating the photon flux emitted from one edge of the tiny device climbed steeply before falling, tracing a shape like a shark's tooth which he had seen many times before. But then the line did something new. It climbed much higher, saturating his detector. Light amplification. Ahn's device was lasing!

Quantum dots are nanoparticles made up of somewhere between 100 and a few hundred thousand atoms of a semiconducting material, such as cadmium selenide. Their allure to science lies in their size. They're essentially zero dimensional—so tiny that they exhibit quantum behavior. Over the past two decades, scientists have harnessed quantum dots' potential for everything from solar windows— semitransparent sunlight collectors that can be applied to glass—to biomarkers that, when paired with antibodies, can tag and illuminate individual cancer cells in vivo. Major electronics manufacturers now layer all different sizes of quantum dots over LED (light-emitting diode) panel screens to create displays with unmatched color purity. "Quantum dots are bridging the gap between virtual reality and reality," says Ahn. They are making the digital world look deceptively like the real world.



Los Alamos researchers Namyoung Ahn (upper -left) and Victor Klimov (lowerright).

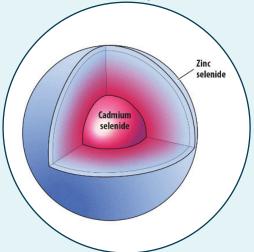
For many quantum dot researchers, the dots' greatest allure lies in their potential to lase. If scientists could build a device around quantum dots that would capture and circulate the photons emitted by the inverted medium, they could produce laser oscillations, which in turn could produce an intense, highly directional, spectrally narrow-band beam of light.



The tiny specs of matter called quantum dots can be tuned to emit light at specific wavelengths. That's just one quality that makes them valuable in a range of technology applications.

A discovery, made in 2018 by Klimov and postdoctoral researcher Jaehoon Lim, led Klimov

to believe that it was possible to get quantum dots to lase through electrical excitation. Lim had used continuously graded dots to demonstrate devices that produced optical gain under electrical excitation. This 2018 discovery had started from work on so-called alloyed quantum dots conducted by postdoctoral



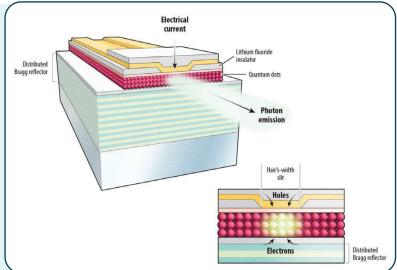
The key to creating quantum dots with a long-lived optical-gain state was to change the dots' composition. This redesign was a leap toward the successful creation of a device that could make quantum dots lase through electrical excitation. researchers Lim and Wan Ki Bae in 2013. In those structures, Lim and Bae retained the cadmium selenide core found in most of the traditional quantum dots but surrounded it by a continuously graded cadmiumselenide-sulfide alloy, with pure cadmium selenide at the core surface gradually transitioning to pure cadmium sulfide on the periphery. This "grading" approach allowed the researchers to suppress so-called Auger recombination—a harmful process—whereby the energy of injected electron-hole pairs dissipates as heat instead of being released as light. Even stronger Auger decay suppression was achieved with the next generation of the engineered quantum dots wherein a cadmium-selenide core was enclosed into a continuously graded cadmium zinc selenide shell. These structures, realized around 2018, allowed LANL researchers to achieve an important milestone—demonstration of optical gain, that is, light amplification with electrically stimulated quantum dots.

With this development, work continued toward lasing with dots. The next challenge was to overcome device overheating and eventual breakdown at high current densities required for laser action. This

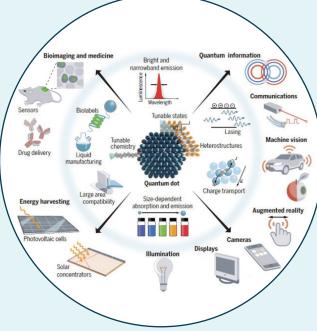
challenge was tackled by Heeyoung Jung, another postdoc in the Klimov team. Initially, Jung concentrated on a "current-focusing" approach when an electric current was delivered to the quantum dots via a small aperture in an insulating interlayer separating a charge injecting electrode from the gain medium. Later, he combined current focusing with pulsing electricity through the device instead of a more continual pumping of electricity. In the "pulsing" approach, a device had a chance to cool between short sequential electrical pulses which allowed Jung to realize unprecedented current densities of more than 1000 Ampere per square centimeter. The result was optical gain for photons with a wide range of wavelengths spanning from red to orange and further yellow.

By 2021, many of the challenges facing Klimov and his team had been solved, however the ability to lase was still eluding them. The team went back to decades of research, including a 1976 paper that introduced the idea of a Bragg reflection waveguide- a way to direct light by elements external to the device. After

reading the almost 50-year-old paper, the Los Alamos researchers got the idea that they could concentrate the photons where they wanted them—in the quantum dot layer-by building their device on top of a so-called distributed Bragg reflector: a stack of transparent layers, made of two materials, that each bent light in different ways. The approach allowed them to steer photons away from all the optically absorbing chargeconducting layers. With this idea in hand, instead of using a glass substrate as he'd always done, Ahn assembled his device on a stack of 20 dielectric layers of alternating refractive indices. Together with the silver mirror on top of the device, which also acted as a hole-injecting electrode, these layers formed a reflection waveguide that would concentrate light in the quantum dot layer and steer it toward the device's edge. Once the device was constructed last April, researcher Clément Livache took spectroscopic measurements and confirmed for the first time that the optical gain overwhelmed optical losses.



The electrically stimulated quantum dot laser that Klimov and his team built. Electric current enters from the top and passes through a narrow silver plate placed perpendicular to a hair's-width slit in the lithium fluoride insulator. This overlap focuses the electricity into a tiny area of less than one-hundredth of a square millimeter. After the focused current hits the quantum dot layer, photons are replicated and then pushed by the constructive interference created by the distributed Bragg reflector out the side of the device.



Quantum dots feature widely tunable and distinctive optical, electrical, chemical, and physical properties. They span energy harvesting, illumination, displays, cameras, sensors, communication and information technology, biology, and medicine, among others. Ahn took the device to his test station and observed all the signatures of light amplification, or single-pass laser action. They had produced a proof of principle for solution-processable laser diodes, a result pursued for decades by researchers worldwide.

Ahn, Livache, and Klimov are now well into the process of patenting their design. And the Klimov team has already moved on to the next steps: working to show that their lasing devices can produce single wavelengths of light and that they can operate on silicon chips, as opposed to glass. With the economic and political prominence of silicon chips rising, the timing couldn't be better. Over the past year, the Biden administration has put more than 50 billion dollars toward the research, development, and manufacture of silicon chips with the 2022 Chips Act. And a recent U.S. trade ruling restricted

the 2022 Chips Act. And a recent U.S. trade ruling restricted international access to American-made semiconducting chips, a move that's likely to produce a surge of interest in alternatives to conventional microelectronic chips. Quantum dot lasers are one of these alternatives which can facilitate a leap toward a next generation of computers powered by something far faster, far more

efficient, far more abundant, and far more powerful than 1s and 0s: light. Read the full article <u>here</u>.

Decades of Dots

A BRIEF GLIMPSE INTO LDRD'S INVESTMENTS IN QUANTUM DOTS RESEARCH





Acknowledgements:

Publication Review

Laura Stonehill Jacob Waltz

Publication Editor Lexi Tyler

Team Contributors

Carole Steward Debora Wagner Epolito Ulibarri Joany Babilonia Lauren Harris Megan Wohlberg Stephen Schultz







LA-UR-24-22509