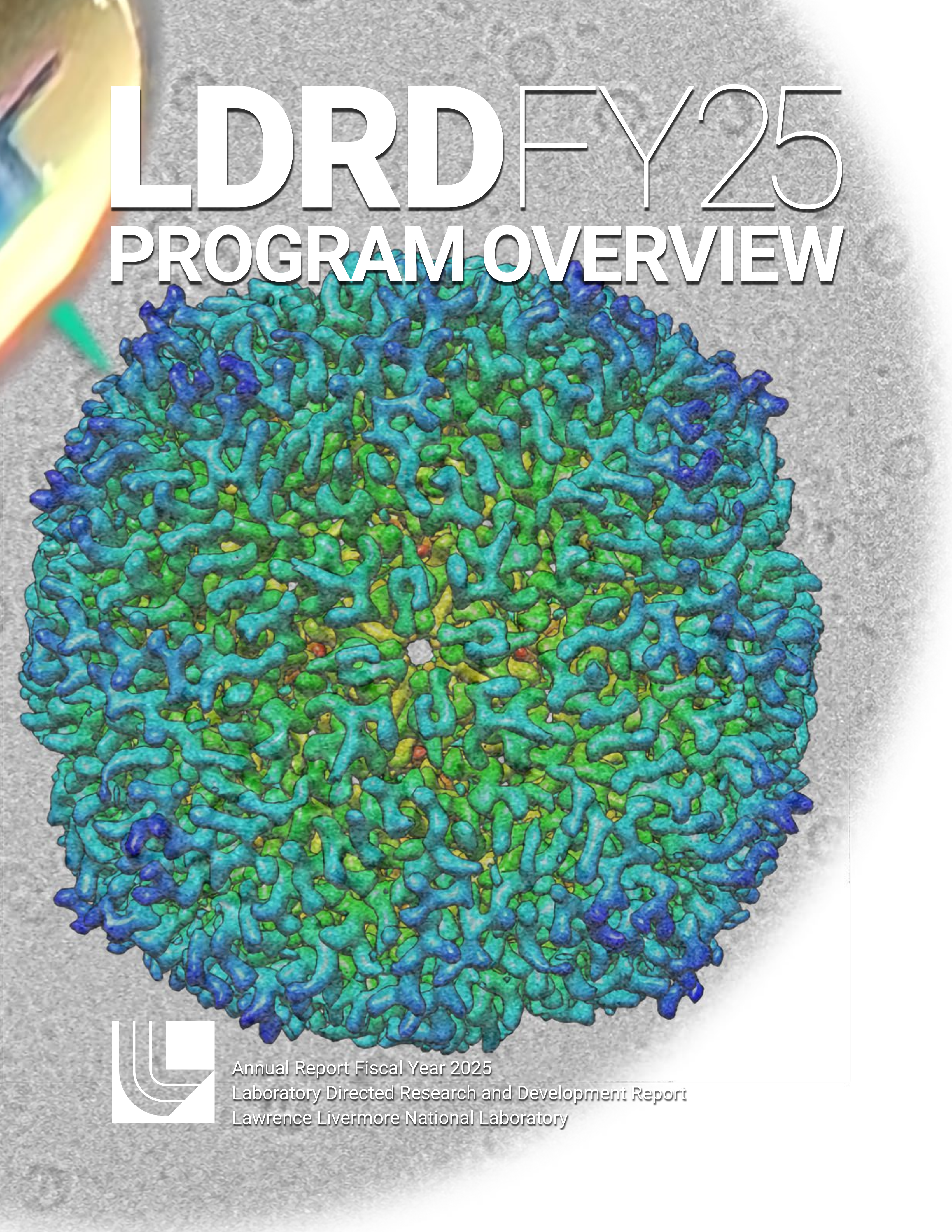
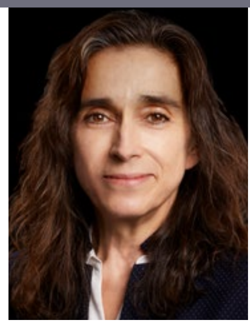
LDRD FY25
PROGRAM OVERVIEW



Annual Report Fiscal Year 2025
Laboratory Directed Research and Development Report
Lawrence Livermore National Laboratory

Director's Statement



As Lawrence Livermore National Laboratory's (LLNL's) Laboratory Directed Research and Development (LDRD) program enters its fifth decade of leading-edge research and development, its impact and importance have never been stronger. The program continues to advance strategic investments in pioneering science, technology, and engineering, ensuring LLNL will be ready to deliver on our mission as it evolves over the coming decades. Investing in LDRD research, and the people who perform this critical work, gives LLNL the ability to sustain our role as a leader in the Department of Energy and National Nuclear Security Administration enterprise.

The LDRD program enables high-risk, high-payoff research that anticipates emerging threats and future mission needs. By nurturing the ingenuity of the Lab's greatest asset, its people, LDRD funding advances not only our research but also grows and nurtures our workforce: engaging future innovators with student mentoring, challenging postdoctoral researchers to apply their skills to support national security, and strengthening the leadership skills of early career staff.

This annual report documents how LDRD investments advance LLNL's science, technology, and engineering across our mission space. To assess LDRD's impact we track both short and long-term metrics such as peer-reviewed publications, number of students, or professional fellows. In addition to reviewing these metrics, I encourage you to delve deeper into the breadth of science and technology that illustrate the strategic value of this research portfolio.

For instance, a recent exploratory research project used advanced manufacturing to construct miniaturized three-dimensional ion traps for a quantum computer with reduced quantum error rates to enable applications that address national security missions and support basic science. Another project has delved into studying detonation by examining deflagration to enhance the safety and security of the nuclear weapons stockpile. LDRD researchers are also deploying AI agents on two of the world's most powerful supercomputers to automate and accelerate inertial confinement fusion experiments. Other teams are delivering more accurate optical constants to enable improved validation for aluminum to advance atomic and molecular physics models. LDRD-driven discoveries of how metals deform under extreme conditions strengthen our ability to model and design materials for demanding national security environments.

National security challenges are increasingly complex and continuously evolving. LDRD focuses our most innovative science and technology on these challenges, ensuring the Laboratory is developing creative, forward-leaning solutions for our nation and the world. The following pages feature highlights of published scientific advances, patents, and honors that stem from LDRD investments. As you read this report, I hope you will understand how these investments position the Laboratory, and our partners, to meet the demands of the decades ahead.

Kimberly S. Budil
LLNL Director

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Contents

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Program Description

The LDRD program's targeted investments allow LLNL to develop cutting-edge capabilities and foster innovation in key programmatic areas.

Mission Alignment

Congress established the Laboratory Directed Research and Development (LDRD) program in 1991 to foster cutting-edge scientific and technical vitality at U.S. Department of Energy (DOE) laboratories. The LDRD programs at each laboratory are a unique resource, providing funding for critical research aimed at addressing today's needs and tomorrow's challenges. LLNL's program addresses DOE objectives, while also aligning with National Nuclear Security Administration (NNSA) mission objectives and the Laboratory's own strategic priorities.

As articulated in DOE Order 413.2C, the LDRD program serves to:

- Maintain the scientific and technical vitality of the laboratories.
- Enhance the laboratories' ability to address current and future DOE/NNSA missions.
- Foster creativity and stimulate exploration of forefront areas of science and technology.
- Serve as a proving ground for new concepts in research and development.
- Support high-risk, potentially high-value research and development.

ALIGNMENT WITH NNSA MISSION OBJECTIVES

A strategic framework — created jointly by NNSA, LLNL, and the other NNSA laboratories — articulates the focus of LDRD programs at NNSA laboratories. LDRD investments support the following NNSA objectives:

- **Technical Vitality**. Develop innovative capabilities that are required to respond to emerging national security challenges.
- **Mission Agility**. Enable agile responses to national security challenges by investing in research and development at the forefront of mission-critical science and technology.
- **Workforce Development**. Recruit, develop, and retain the best and brightest staff, who can help us creatively address tomorrow's dynamic mission needs.

ALIGNMENT WITH LABORATORY MISSIONS

In addition to aligning our LDRD investments with DOE and NNSA objectives, we ensure that our LDRD program supports mission priorities articulated in LLNL's annual strategic investment plan. Institutional goals are established and updated through a planning process where multidisciplinary teams identify:

- Mission-related challenges or areas of interest for high-priority research.
- The Core Competencies that support this high-priority research.
- The scientific and technological needs to address those challenges and enhance related competencies.
- Key topics in fundamental research.

Program Oversight

Day-to-day oversight of our program is provided by LDRD Program Director Elizabeth Wheeler. Overall program oversight extends beyond the LDRD program office to include the LLNL Director and the LLNL Deputy Director for Science and Technology, along with the Laboratory's scientific and programmatic leaders. This Laboratory team works closely with NNSA's Livermore field office, NNSA's LDRD program leaders, and LDRD program leaders at the DOE.

At the programmatic level, LDRD portfolio management at Livermore is structured to assure alignment with DOE, NNSA, and Laboratory missions. Designated LDRD points of contact for each of the Laboratory's strategic investment areas provide input regarding LDRD investment priorities to Livermore's senior leadership team. These points of contact also advise applicants for LDRD funding regarding the alignment between proposed research and evolving mission needs at our Laboratory.

In addition, programmatic leaders and science and technology leaders spend a combined 3,000 hours in a rigorous peer-review process of all proposals for LDRD funding. They evaluate the scientific and technical impact of each proposal, as well as its technical content and project execution plan. NNSA reviews and concurs on funding decisions. In addition, funded projects are periodically reviewed by senior staff to ensure technical success and continued alignment with mission objectives.

PERFORMANCE ASSESSMENT

The LDRD program achieves continuous improvement through internal and external reviews of the program, along with oversight of each LDRD research project.

Representatives from LDRD programs at each NNSA laboratory regularly participate in working groups to share best practices and discuss strategies for tracking the long-term impact of LDRD investments.

To assess continued LDRD performance, the LDRD program tracks a suite of short-term and long-term metrics. These performance metrics can be found in the Program Value section of this report and address scientific publications, intellectual property, collaborations, and support for early-career staff. Also included are NNSA-guided metrics for assessing the long-term impact of LDRD on laboratory staff and capabilities. Our report also includes performance indicators specified by DOE's Director of LDRD programs, in accordance with DOE Order 413.2C.

PATRICIA FALCONE
LLNL Deputy Director for Science and Technology
"LLNL's *Investment Strategy for Science and Technology* is updated annually to reflect evolving mission needs, under the guidance of LLNL's Deputy Director for Science and Technology. It sets the strategic context for LLNL's annual call for LDRD proposals, and it serves as a resource for investigators as they articulate the ways their proposed research aligns with at least one of these investment priorities."

ELIZABETH WHEELER
LDRD Program Director
"LDRD-funded projects are critical to advancing a broad range of science and technology areas, often seeding the foundation for new programmatic directions," said Elizabeth Wheeler, director of Livermore's LDRD Program. "LDRD projects also continue to develop our workforce pipeline from onboarding students and postdoctoral researchers to establishing collaborations with universities and other research institutions — helping to ensure the long-term technical vitality of our Laboratory."

Program Description

FY25 INVESTMENTS

247 PROJECTS

$177M TOTAL FUNDING

Investment Portfolio

LDRD investments span a broad range of research topics, helping to ensure that LLNL supports innovation in key programmatic areas. Funded projects advance our emerging technologies and evolving mission spaces. We also invest in the core capabilities and programmatic areas that undergird our Laboratory's technical vitality and mission agility.

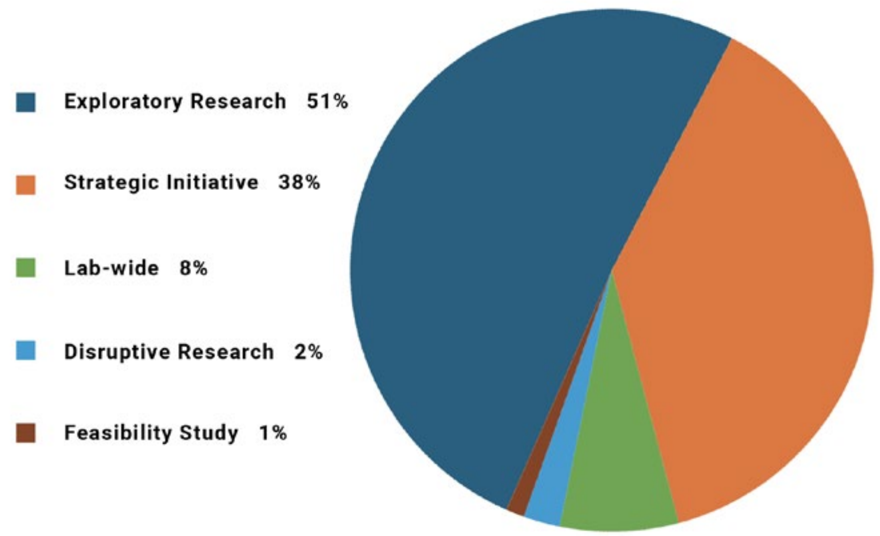
For fiscal year 2025 (FY25), we carefully structured Livermore's LDRD investment portfolio to promote the short-term objectives and long-term goals of DOE, NNSA, and our Laboratory. The key metrics presented here regarding our FY25 investment portfolio reflect this structure, including how funds are distributed across the program's five types of projects and 11 research categories. By strategically selecting the types of projects we fund, along with the amount of funding invested in each project, we help ensure a strong program portfolio.

FUNDING BY PROJECT TYPE

Livermore's LDRD program includes five types of projects. Each one has a distinctive purpose, duration, and funding limit. For example, our one-year feasibility studies support relatively brief investigations of a specific technical approach. These types of projects can be launched mid-year to rapidly respond to an emerging challenge. Other types of projects span up to three years, often involving collaborators and research that tackles a broader scope of challenges.

PROJECT TYPE	FY25 PROJECTS FUNDED	PROJECT AIM
Exploratory Research (ER)	159	Address a specific research challenge or enhance a core competency.
Feasibility Study (FS)	17	Determine the viability of a new way to address a mission-relevant challenge.
Lab-wide (LW)	43	Conduct innovative basic research and technology to enable out-of-the-box thinking.
Strategic Initiative (SI)	20	Make significant progress addressing a mission-relevant challenge from a multidisciplinary perspective.
Disruptive Research (DR)	8	Pursue novel ideas with the potential to overturn fundamental paradigms or create new research directions.

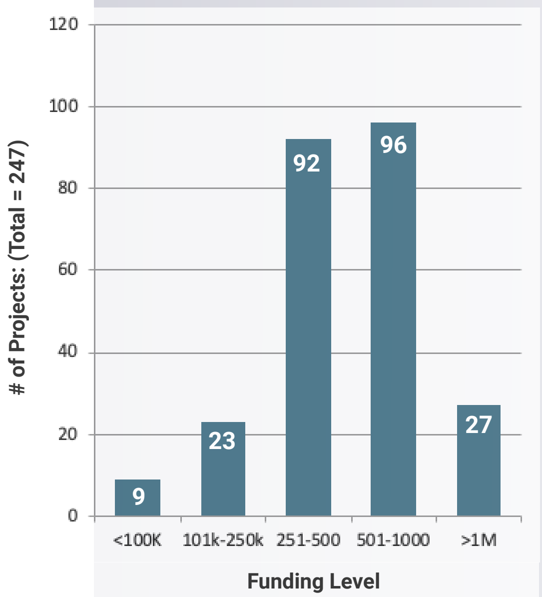
PERCENTAGE OF FUNDING BY CATEGORY



PROJECTS BY FUNDING LEVEL

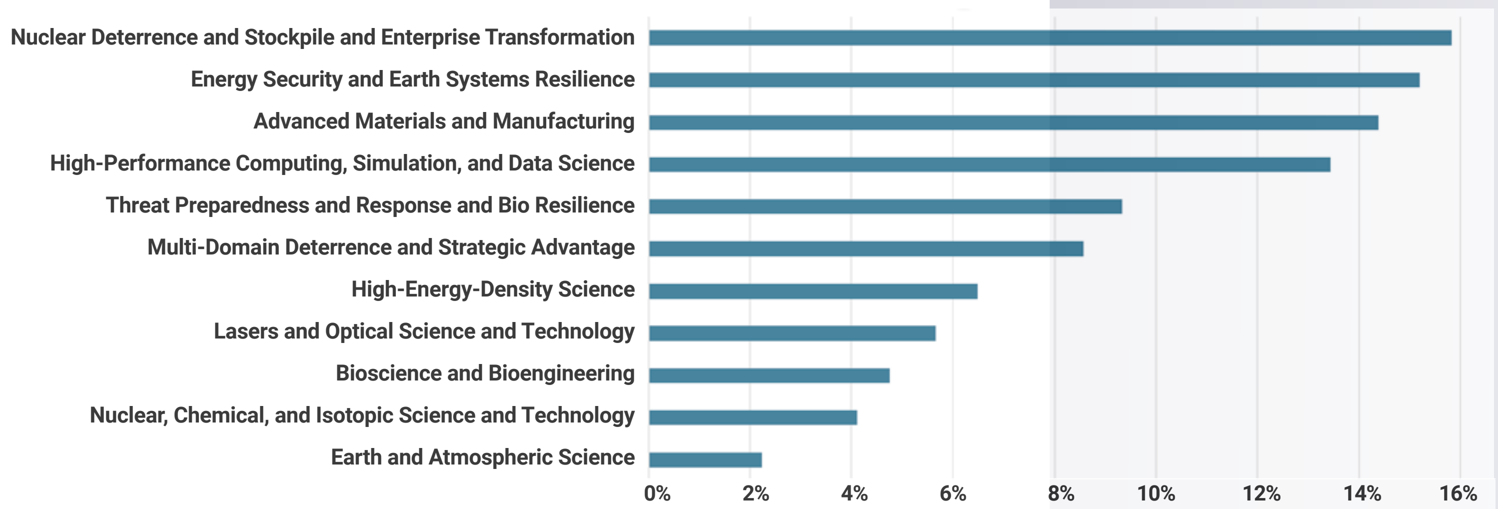
Average funding level per project: $715,150

Our Laboratory's investment strategy includes the flexibility to fund projects at varying dollar amounts, depending on the project scope. This chart presents data on the number of projects funded in FY25, distributed across five funding levels. The largest number of projects (96) fell in a higher funding range, receiving between 501K and 1000K per project. A smaller number of projects received less than $100K in funding (9 projects), or more than $1M in funding (27 projects).



FUNDING BY RESEARCH AREA

Every LDRD project is assigned to at least one of the Laboratory's research areas in the LDRD investment portfolio. The categories include four Mission Areas and seven Core Competencies—capabilities that enable us to conduct high-priority, mission-relevant research.



Program Value

73 unique institutions were involved in formal collaborations as part of LDRD-funded research teams in FY25.

From publications to intellectual property to long-term impact, LDRD is a major contributor to scientific and technological accomplishments.

Collaborative Explorations

External collaborations are essential to the innovative research that takes place at LLNL, including LDRD-funded projects. By collaborating with other national laboratories, academia, and industry, our investigators can engage with experts from other institutions and access world-class experimental facilities.

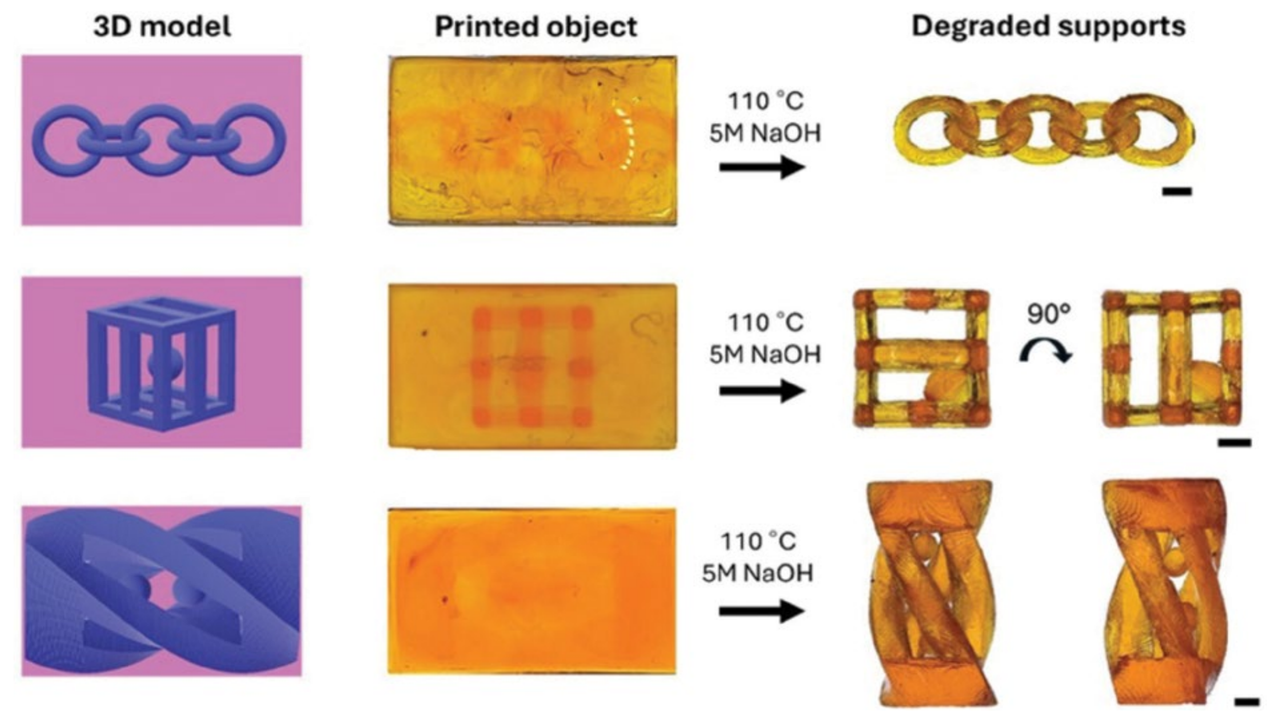
The following table provides our most recent data regarding formal collaborations, which we define as LDRD-funded projects where an external collaborator received LDRD funds from LLNL. In addition, our investigators frequently participate in informal collaborations with researchers at other institutions, which often involve joint scientific publications. Both types of collaborations are a key indicator of the broad intellectual engagement that is a hallmark of LLNL's research environment.

COLLABORATIONS	FY21	FY22	FY23	FY24	FY25
LDRD-funded projects with one or more formal collaborations	88	79	81	79	75
Total percent of projects with formal collaborations	33%	32%	30%	31%	30%

LLNL TEAM TACKLES SUPPORT STRUCTURE BOTTLENECKS WITH DUAL-WAVELENGTH 3D PRINTING

Lawrence Livermore National Laboratory researchers have developed a novel 3D printing technique that uses light to build complex structures, then cleanly dissolves the support material, expanding possibilities in multi-material additive manufacturing (AM).

In 3D printing, traditional supports often add time, waste and risk to the process, especially when printing intricate parts. But in a new study published in *ACS Central Science*, an LLNL team — in collaboration with University of California, Santa Barbara (UCSB) researchers — outlines a "one-pot" printing approach that uses two light wavelengths to simultaneously create permanent structures and temporary supports from a single resin formulation.



A "one pot," light-based 3D printing process developed by LLNL researchers addresses a longstanding challenge in additive manufacturing: how to fabricate suspended or overhanging features without scaffolding requiring manual removal, a hurdle to widespread adoption of Digital Light Processing printing technologies. (Photos by Isabel Arias Ponce/LLNL)

The method addresses a longstanding challenge in AM: how to fabricate suspended or overhanging features without cumbersome scaffolding requiring manual removal, which is a key hurdle to widespread adoption of Digital Light Processing (DLP) 3D printing technologies.

"This work adds another option to the growing range of multi-material printing possibilities," said principal investigator and LLNL staff researcher Maxim Shusteff. "Using multiple materials is critical to many manufacturing processes, and that's been hard to accomplish using 3D printing. And manually removing supports printed from the same material is one of the bottlenecks preventing the use of DLP in production activities and hurting part accuracy — dissolving a sacrificial material is much more automation-compatible and less cumbersome."

One of the study's key innovations lies in a custom-built, dual-wavelength negative imaging (DWNI) DLP printer, patented by co-author and LLNL engineer Bryan Moran. The system uses a single digital micromirror device to project both ultraviolet (UV) and visible light at the same time, each triggering a different chemical reaction. The UV light solidifies the final epoxy structure, while the visible light cures a degradable thermoset designed to dissolve post-printing.

After thermal postprocessing, the printed objects are placed in a basic water-based solution, where the supports gently dissolve, leaving the primary structure intact with no damage or residue. The team successfully demonstrated free-floating designs including interlocked rings and a ball-in-a-cage — shapes that are difficult or impossible to produce with conventional layer-by-layer methods.

The approach offers practical advantages: reduced print time, minimal material waste and improved resolution. It also avoids the need to swap resins mid-print, a common obstacle in multi-material 3D printing, researchers said.

"Our one-pot embedded printing approach improves the fidelity of unsupported, free-floating structures, such as overhangs and cantilevers, by using degradable supports that act as temporary scaffolds to prevent collapse and misalignment during fabrication," said first author Isabel Arias Ponce, a UC National Laboratory Fees Graduate Scholar and soon-to-be LLNL materials engineer. "Additionally, mobile components — such as hinges and interlocking systems — could be fabricated in place by simply patterning a degradable interface between multiple parts. This would eliminate the need for manual assembly and enhance production efficiency."

Co-authors include former LLNL Postdoctoral Fellow Sijia Huang, currently an assistant professor at the University of Utah; and Professor Craig Hawker of UCSB.

LDRD Project Title:
Designing Semi-Crystalline Photopolymers via Solid-State Photopolymerization
Principal Investigator:
Maxim Shusteff and Sijia Huang
LDRD Project:
25-LW-116
https://doi.org/10.1021/acscentsci.5c00337

Intellectual Property

Year after year, the percentage of patents and copyrights issued for LDRD research go far beyond the program's 6% funding level. As illustrated in the following tables, LDRD-funded work has been key in developing more than half of the Laboratory's patents, one-third of the Laboratory's copyrights (chiefly computer codes), and more than half of the Laboratory's records of invention. Patent filings include international awards.

LDRD-FUNDED WORK HAS PLAYED A KEY ROLE IN DEVELOPING MORE THAN 50% OF THE LABORATORY'S PATENTS.

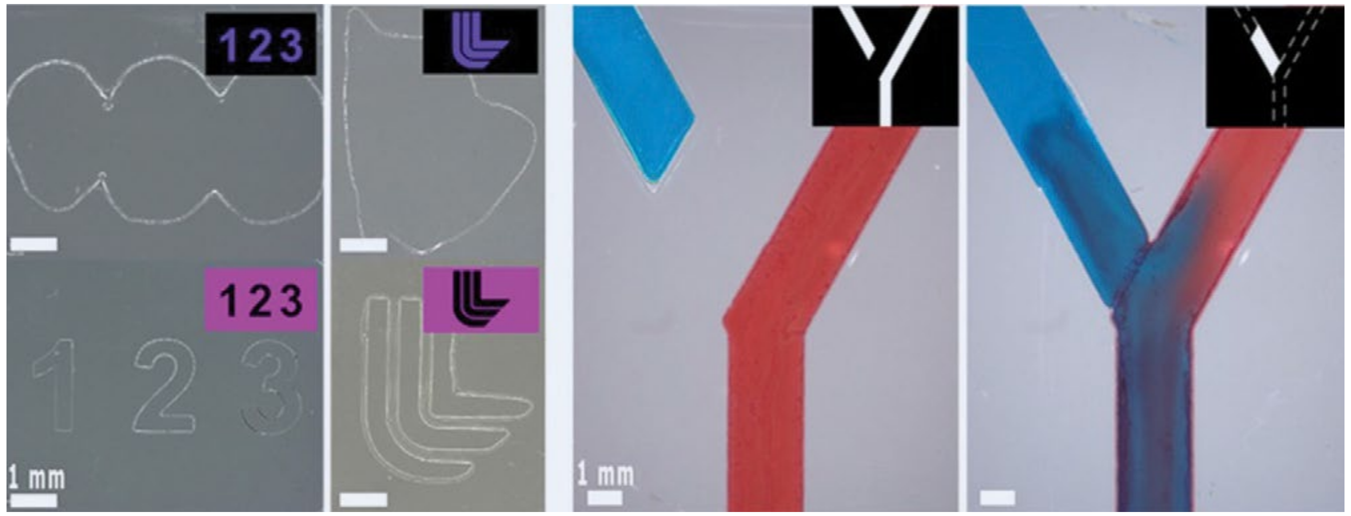
PATENTS	FY21	FY22	FY23	FY24	FY25
All LLNL patents	166	166	197	200	147
LDRD patents	96	103	116	126	88
LDRD patents as a percentage of total	58%	62%	58%	63%	61%

COPYRIGHTS	FY21	FY22	FY23	FY24	FY25
All LLNL copyrights	125	142	166	201	238
LDRD copyrights	42	47	44	66	76
LDRD copyrights as a percentage of total	34%	33%	26%	33%	32%

RECORDS OF INVENTION	FY21	FY22	FY23	FY24	FY25
All LLNL records	89	70	120	119	88
LDRD records	53	40	64	61	42
LDRD records as a percentage of total	60%	57%	53%	51%	48%

LDRD-funded work continues to play a key role in developing more than 50% of the Laboratory's patents.

UNIQUE RESIN ALLOWS 3D-PRINTING METHOD TO ADD AND SUBTRACT



Demonstrations of a new corrective manufacturing technique. In the left panel (a), low resolution printed shapes are shown at top and corrected shapes are shown at bottom. In the right panel (b), hybrid manufacturing is used to correct a gap in a fluidic structure. (Credit: Howard et al.)

LDRD Project Title:
Volumetric Subtractive Manufacturing
Principal Investigator:
Liliana Dongping Terrel-Perez
LDRD Project:
24-LW-069
https://doi.org/10.1002/admt.202500997

Additive manufacturing, or 3D printing, is normally a one-way street. In a digital light processing (DLP) printer, a structured pattern is projected onto a layer of liquid resin, which cures and solidifies. This builds an object up, layer-by-layer. But if the print isn't exactly right, there's no easy way to fix it after the fact: it usually ends up in the trash.

In a new study, published in *Advanced Materials Technologies*, researchers at LLNL developed a hybrid additive and subtractive manufacturing system with a unique resin that enhances traditional 3D printing by introducing dual-wavelength behavior. Under blue light, the resin cures and hardens. Under ultraviolet light, it degrades back into a liquid. The hybrid printing system enables corrective manufacturing, provides improved print resolution and allows for upcycling and recycling of parts.

"Imagine if a company needed a part to fit a certain machine but it's a prototype and they're not quite sure what they want," said LLNL scientist and author Benjamin Alameda. "They could theoretically print with our resin. And if there were defects or something they wanted to change about it, they don't have to print a whole new part. They could just shine another wavelength on it and modify the existing part. That's useful and less wasteful."

The patented resin technology is available for commercialization through LLNL's Innovation and Partnerships Office (IPO). It allows all light-based printing systems to create more intricate, detailed parts with higher resolution, to smooth surfaces and correct errors, as well as to add and remove temporary support structures. The technology — produced using unique LLNL facilities, capabilities and expertise — can be licensed by advanced manufacturing companies and used in existing 3D printers to save time and materials cost by enabling editable, recyclable 3D prints.

The resin is the key to the success of this dual-function printing: the authors optimized each component of its chemistry. Blue light causes the molecules in the resin to combine into a cross-linked network, a standard technique in 3D printing. In a new twist, ultraviolet light generates acid in the resin. The molecules are specifically tailored to respond to acid, breaking back down into a liquid.

Balancing the stability and degradability was a challenge. The team designed the resin to harden and degrade quickly, but not so quickly that it would degrade on its own. They noted that standard coatings can prevent parts from breaking down in the sun's natural ultraviolet radiation.

Going forward, the scientists are further expanding the capability of this hybrid manufacturing by integrating on-machine metrology and feedback control to automatically and autonomously correct the print errors on-the-fly.

"Once we see there are printing errors, we can adaptively modify the projection images to correct those errors on-the-fly, which enables a true adaptive manufacturing. Besides DLP printing, we are also planning to transfer this method to volumetric additive and subtractive manufacturing, which shines light to a rotating vial of resin and fabricates a 3D part all at once," said author and LLNL scientist Liliana Dongping Terrel-Perez.

The project was funded by LDRD office and led by Liliana Dongping Terrel-Perez. In addition to Alameda and Schwartz, team members include Holden Howard, Martin De Beer and Magi Yassa.

Tracing Impact to LDRD Roots

Throughout this section, we mention “LDRD roots.” Much discussion with principal investigators has transpired 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 at least one LDRD project needed to occur for the accomplishment to take place. In other words, if one can identify an LDRD project that was critical to the accomplishment, then it is considered to have LDRD roots.

Scientific Publications

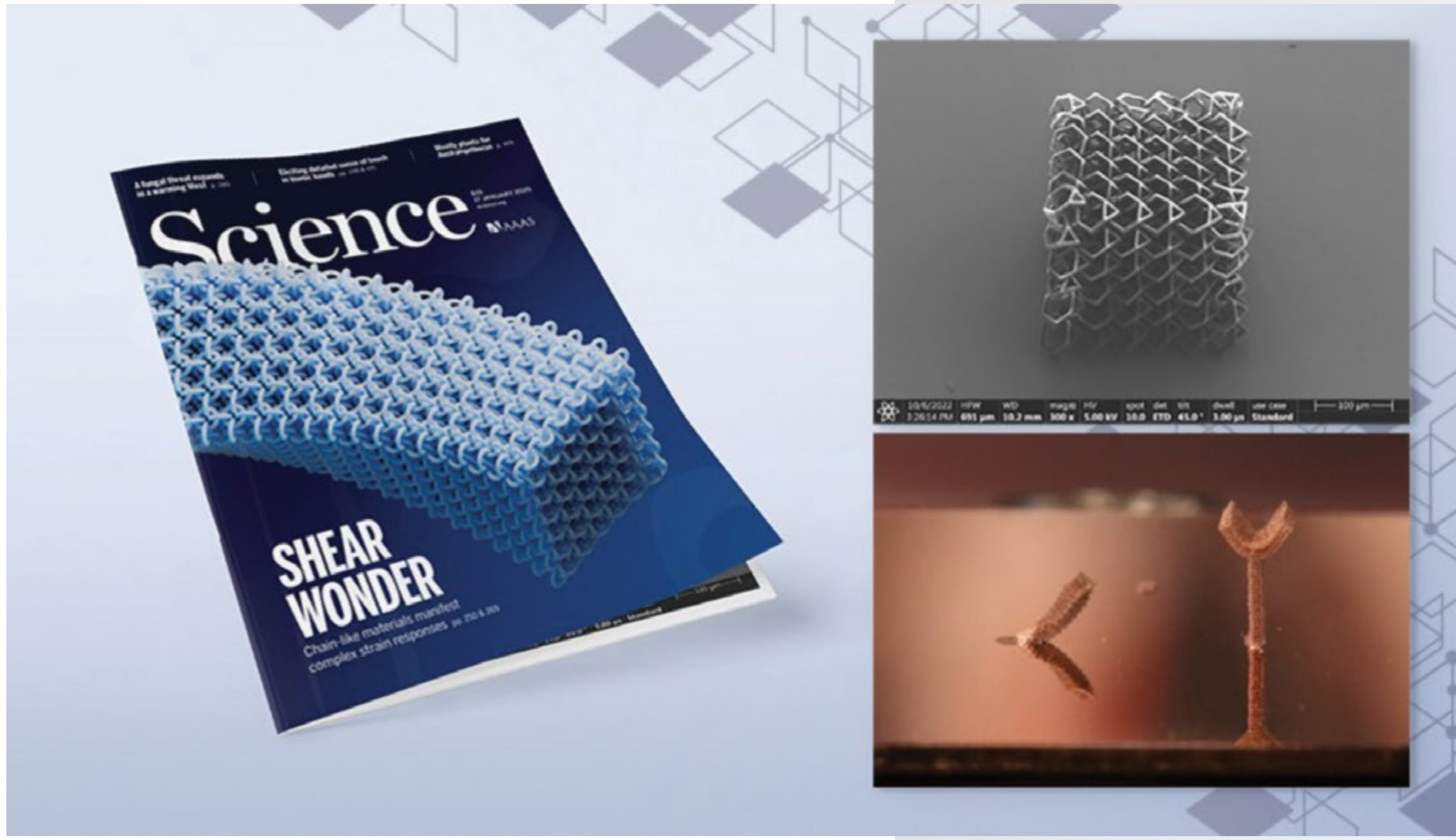
Laboratory scientists and engineers publish more than a thousand papers each year in a wide range of peer-reviewed journals, of which LDRD-funded work accounts for a large portion. The numerous publications made possible through LDRD-sponsored research help the Laboratory maintain a strong presence in the broader scientific community, extending the impact of LDRD research beyond the DOE mission space into the wider scientific arena. In addition, the impact of these publications documenting LDRD project results extends long after articles appear in the journals, increasing the value of LDRD investments in these projects.

PROGRAM VALUE

By almost any measurement, the LDRD program contributes far more in publications, intellectual property, collaborations, and recruitment of postdoctoral researchers — dollar for dollar — than any other program at the Laboratory.

JOURNAL ARTICLES	FY21	FY22	FY23	FY24	FY25
All LLNL articles	1,256	1,149	1,218	1,004	1,079
LDRD articles	509	490	495	409	407
LDRD articles as a percentage of total	41%	43%	41%	41%	38%

LLNL RESEARCHERS EXPLORE FUTURE OF RESPONSIVE 3D-ARCHITECTED MATERIALS



Researchers from Lawrence Livermore National Laboratory, the California Institute of Technology and Princeton University have introduced a revolutionary new class of materials known as 3D polycatenated architected materials. These intricate structures can behave with both solid and liquid-like properties and have the potential to impact industries ranging from engineering to medicine. (Graphic: Dan Herchek/LLNL. Photos: Xiaoxing Xia. Cover image reprinted with permission from AAAS).

In the evolving fields of materials science and 3D printing, engineers at Lawrence Livermore National Laboratory are exploring novel ways to create materials and structures that adapt and respond to their environments.

A recent study featured on the cover of *Science*, conducted in collaboration with the California Institute of Technology (CalTech) and Princeton University, has introduced a revolutionary class of materials known as 3D polycatenated architected materials (PAMs). These intricate structures can behave with both solid and liquid-like properties and have the potential to impact industries ranging from engineering to medicine.

“Polycatenated” describes how these new architected materials are built-multiple interconnected loops or cages form a flexible and resilient framework, akin to chain mail armor-enabling dynamic responses to external forces. When subjected to specific stressors, these networks show a transformative capability, expanding, contracting or morphing into entirely new shapes.

“Architected materials can be designed and 3D printed to have specific internal structures that define their properties but are generally rigidly connected repeating units-the interaction between neighboring units is limited," explained LLNL staff scientist and co-corresponding author Xiaoxing Xia. "PAMs, however, have interlocked building blocks that cannot be separated but can move with much greater freedom compared to rigid lattices. This gives them the ability to behave like both a liquid and a solid under different conditions."

THE SCIENCE BEHIND PAMS

The team, including LLNL engineers Xia and Anna Guell Izard, conducted experiments examining PAMs' mechanical properties under various conditions. One key finding was gravitational relaxation where PAMs change shape in response to gravitational forces, suggesting applications in stimuli-responsive materials, energy-absorbing systems and morphing architectures, particularly in low or zero-gravity environments.

"In space, a little bit of electrostatic interaction can expand a large, interlocked network, potentially shielding a space station or satellite or deploying flexible solar panels or telescopes," Xia said. "When submerged in liquid, PAMs-especially micro-PAMs-remain highly mobile with minimal influence of gravity, making them useful for micro-robotic or bio-implantable applications."

Additionally, PAMs respond differently depending on their orientation along specific crystallographic axes, the researchers reported. When tested on a flat surface and oriented along multiple axes, they displayed distinct relaxed outline shapes, highlighting the critical role of internal structure in mechanical response.

The researchers also demonstrated PAMs' length-scale-independence, fabricating them at both macro and microscale levels while maintaining consistent mechanical responses. This scalability suggests the PAMs' behavior can apply to structures ranging from microscopic medical devices to large-scale architectural components, they reported.

LDRD Project Title:
Large-Scale, Two-Photon, Three-Dimensional Printing Enabled by Metaoptics
Principal Investigator:
Xiaoxing Xia
LDRD Project:
22-ERD-004
https://www.science.org/doi/10.1126/science.adr9713

FUTURE VISION AND THE ROLE IN ENERGY ABSORPTION

Researchers said PAMs could impact engineering by enabling lightweight, durable structures that can withstand extreme conditions. Aerospace engineers, for instance, could design aircraft components that balance strength and efficiency. Additionally, the PAMs ability to absorb energy, redistribute stress and deform predictably could be ideal for protective gear such as helmets and body armor.

"Normally lattice structures are used for lightweight applications; when one unit is fractured, cracks can propagate easily, causing catastrophic failure," Xia said. "Since PAMs are not rigidly connected, elastic or shock waves struggle to transmit from one unit to another, making them excellent for energy absorption under impact. Also, their shear-thinning behavior — solid-like under zero or low frequency vibration but liquid-like under high frequency — could also mitigate vibrations mitigation during rocket launches."

In the medical field, PAMs could enhance prosthetics and implants, adapting shape and stiffness to a user's movements for a more natural experience. They could enable precise drug delivery systems by altering their shape to release medication where needed, the researchers said.

ELECTROSTATIC RESPONSIVENESS AND SMART MATERIALS

Another notable aspect of the study is the role of electrostatic forces in PAM behavior. The team coated microscale PAM samples with a thin copper layer to enhance electrical conductivity. Xia recalled observing intriguing movement when he placed a micro-PAM in water and later noticed under a scanning electron microscope (SEM) that electron beams charged up the rings, causing them to repel each other due to electrostatic repulsion.

"The rings were shaking a little bit and some rings started to levitate slightly," Xia said. "Because the charge in SEM was minimal, I bought a small Van de Graaff generator, which provided much more charge. Each ring or cage immediately repelled the others, causing the entire structure to expand and stand up due to the electrostatic forces."

This rapid, reversible transformation suggests potential applications in smart systems that react to electrical signals. PAMs could be used in robotics that change shape or stiffness in response to electrical inputs. In wearable tech, they could form the clothing or devices that adjust in real time for enhanced comfort and functionality.

CHALLENGES AND FUTURE WORK

Despite their potential, PAMs face challenges in large-scale production. Variations in fabrication techniques can affect material properties, and micro-PAMs fabrication has proven particularly difficult due to limitations in 3D printing.

"For most 3D printing methods, you cannot print unsupported structures," Xia said. "In the end, we embedded PAMs in thin supporting lattices and used oxygen plasma to remove them — requiring a lot of patience."

To address this, LLNL researchers are developing new printing techniques to streamline fabrication. Songyun Gu, a postdoc in LLNL's Materials Engineering Division, has successfully made larger interlocked networks using a parallel 3D printing setup. Recent mechanical tests done by Guell Izard show these structures exhibit greater toughness and resilience than traditional octet lattices because cracks struggle to propagate, Xia said.

The team continues to investigate PAMs' unique properties and long-term behavior under varying environmental conditions, such as temperature, humidity and chemical exposure, which will help ensure their real-world durability and performance.

The LLNL portion of the work was funded by the Laboratory Directed Research and Development program under Xia's project titled "Large-Scale, Two-Photon, Three-Dimensional Printing Enabled by Metaoptics." Additional funding for the collaboration came from the Gary Clinard Innovation Fund and the Army Research Office.

Other co-authors included first author Wenjie Zhou, Sujeeka Nadarajah, Hujie Yan, Aashutosh Prachet, Payal Pate, Chiara Daraio of Caltech and Liuchi Li of Princeton.

Projects sponsored by LDRD contribute significantly to the recruitment of postdoctoral and early-career researchers at LLNL.

Early-Career Opportunities

STUDENTS AND POSTDOCTORAL FELLOWS

By funding exciting, potentially high-payoff projects at the frontiers of science, the LDRD program attracts top talent in new and emerging fields of science and technology. As shown in the following tables, LDRD investments contribute to the health and robustness of LLNL's student and postdoctoral researcher programs.

STUDENTS	FY21	FY22	FY23	FY24	FY25
Students supported by LDRD	136	149	185	216	203
Percentage of all students	24%	23%	24%	26%	27%

POSTDOCTORAL RESEARCHERS	FY21	FY22	FY23	FY24	FY25
Postdoctoral researchers supported by LDRD greater than or equal to 10% of their time.	208	240	213	234	205
Percentage of all postdoctoral researchers	54%	56%	51%	58%	55%
LDRD postdoctoral researchers converted to full staff	50	72	56	44	48
Percentage of all conversions	82%	77%	70%	66%	76%

PROGRAM VALUE

LDRD provides opportunities to students, postdocs, and early-career staff to set them up for long-term success.

LLNL PHYSICIST COLE PRUITT HONORED WITH EARLY-CAREER ACHIEVEMENT AWARD

LLNL physicist Cole Pruitt is the recipient of the 2025 FRIB Early Career Award in theoretical nuclear physics for his contributions to uncertainty-based nuclear reaction modeling. (Photo: Blaise Douros/LLNL)

Lawrence Livermore National Laboratory physicist Cole Pruitt has been awarded the 2025 Facility for Rare Isotope Beams (FRIB) Achievement Award for Early Career Researchers in theoretical nuclear physics. The national honor recognizes early-career scientists who have made significant contributions to nuclear physics research at or in connection with FRIB.

Pruitt, a staff scientist in LLNL's Design Physics Division, was selected for his work developing uncertainty-quantified optical model potentials, tools that improve predictions of how nuclear reactions unfold, especially in rare, short-lived systems.

"Optical model potentials help estimate the forces that protons and neutrons experience as they move through atomic nuclei during nuclear reactions," Pruitt said. "They're essential for simulating how these reactions behave."

While today's models perform well for stable nuclei, Pruitt's research focuses on improving their reliability for neutron-rich, unstable systems. His postdoctoral work at LLNL introduced uncertainty estimates into these models, making it possible to better predict how elements form in extreme environments such as neutron star mergers.

The approach also helps guide experimental priorities at FRIB by pointing to nuclei where new measurements are most likely to improve model accuracy.

"This is a significant achievement and speaks to Cole's innovative contributions to theoretical nuclear physics," said David Miller, physicist and group leader in the Design Physics Division. "Additionally, recognition by FRIB underscores the caliber of early-career talent here at Livermore."

Pruitt began developing this research framework while earning his Ph.D. in chemistry from Washington University in St. Louis. He joined LLNL in 2019 as a postdoctoral researcher in the Physical and Life Sciences Directorate before becoming a staff scientist in Design Physics, where he continues to contribute to LLNL's nuclear science and national security mission. Pruitt has participated in LDRD team projects focused on nuclear, chemical, and isotopic science and technology.

Professional Fellows

One relevant indicator of advancement and leadership in a scientific 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.

American Physical Society (APS) fellowships are awarded based on scientific merit and impact over an extended period, and the evaluation process relies on nomination and recommendation by peers. As such, data regarding the history of APS fellowships awarded to LLNL physicists provide an important indicator regarding the key role that the LDRD program plays in developing the technical, scientific, and leadership skills of early-career staff. As presented in the following table, in fiscal year 2024 (FY24),100% of the new APS Fellows from LLNL had early-career LDRD experience.

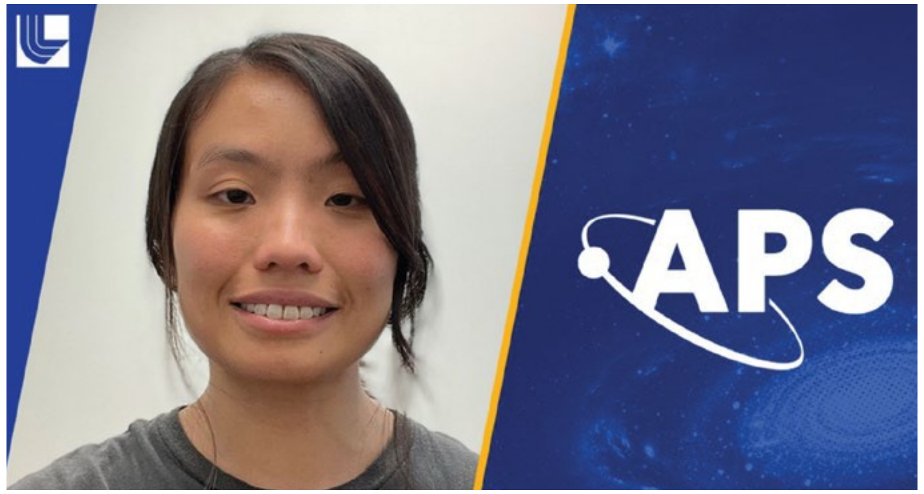
Because the quantity of awards each year is a small number, we also present multi-year statistics. For example, over the last 10 years, more than 90% of the APS Fellows at LLNL had early-career LDRD experience.

	Single-Year Statistics			Multi-Year Statistics		
HISTORY OF APS FELLOWS AT LLNL	FY22	FY23	FY24	FY16-20 (5 YRS)	FY21-25 (5 YRS)	FY16-25 (10 YRS)
Total APS awards	26	2	3	21	10	31
Awards with LDRD roots	20	2	3	20	19	30
% with LDRD roots	77%	100%	100%	90%	100%	97%
Average years from first LDRD experience	16.4	15.5	8.3	18.2	10	15.5

LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

2025 APS FELLOWS AT LLNL

LLNL'S WEI JIA ONG RECEIVES AMERICAN PHYSICAL SOCIETY'S 2025 FREEDMAN AWARD



The American Physical Society has recognized Wei Jia Ong, a staff scientist at Lawrence Livermore National Laboratory, as the recipient of the 2025 Stuart Jay Freedman Award in Experimental Nuclear Physics. (Graphic: Dan Herchek/LLNL)

Wei Jia Ong, a staff scientist at LLNL, has been recognized as the recipient of the American Physical Society's (APS) 2025 Stuart Jay Freedman Award in Experimental Nuclear Physics.

The award is presented annually to an outstanding early-career experimentalist in nuclear physics. Ong was selected for her work "spearheading a multifaceted effort that uses radioactive beams to better understand Type-I x-ray bursts and other astrophysical phenomena through studies of beta decay, nuclear reactions and nuclear masses."

"It is an unbelievable honor to win this award," said Ong. "At the same time, science is not done in a vacuum. I have been extremely fortunate throughout my research career to have had amazing mentors and peers."

Ong's research focuses on nuclear astrophysics, particularly the formation of elements in the cosmos and the nuclear reactions that take place in neutron stars.

The award recognizes Ong's study of x-ray bursts, in which a neutron star siphons and heats material from a companion star. Eventually, the accreted gas becomes hot enough to trigger a thermonuclear explosion on the surface of the neutron star.

Ong joined LLNL as a Lawrence Fellow — a highly competitive postdoctoral position offered at the Laboratory. She also completed several LDRD projects in the area of nuclear, chemical, and isotopic science and technology. She is now a staff scientist in the Nuclear and Chemical Sciences Division.

The APS award was established in 2016 in honor of Stuart J. Freedman, a distinguished experimental nuclear physicist with a devotion to educating and mentoring graduate students and postdoctoral researchers. As the recipient, Ong received $5,000, a certificate, a registration waiver and an allowance for travel to the fall meeting of the APS Division of Nuclear Physics to give an invited prize talk and receive the award.

Long-Term Impact

The LDRD program is an investment in our nation's future, ensuring mission support that is often realized many years after an LDRD-funded project concludes. Recognizing this long-term impact of the LDRD program, we believe it is important to highlight indicators that span multiple years, demonstrating the true impact of LDRD as a national asset.

We collaborated with our colleagues from LDRD programs at other NNSA institutions to identify ways that could best represent the long-term impact of LDRD investments. As each institution issues its LDRD program report for FY25, we present a common set of long-term performance indicators including the content provided below.

DISTINGUISHED MEMBER OF THE TECHNICAL STAFF

One relevant indicator of career advancement in a science and technology field is the recognition of individuals as distinguished members of the technical staff at the institution. Individuals who receive this recognition are identified as being in the top 1% or 2% of the institution's scientific and technical staff, similar to a lifetime achievement award, or in this case, for their contribution to the Laboratory's mission.

At LLNL, appointment as a Distinguished Member of the Technical Staff (DMTS) is reserved for Laboratory scientists and engineers who have demonstrated a sustained history of high-level achievements in programs of importance to the Laboratory, become a recognized authority in the field, or made a fundamental and important discovery that has sustained, widespread impact.

As presented in the following table, a vast majority of these distinguished staff at LLNL had early-career experience with LDRD projects, which helped them develop their scientific, technical, and leadership skills. Please note that the DMTS are not identified every year and the FY25 DMTS call was postponed to Q1 of FY26 so is not included in the summary table below.

	Single-Year Statistics		Multi-Year Statistics		
HISTORY OF DMTS AWARDS AT LLNL	FY22	FY24	FY16-20 (5 YRS)	FY21-25 (5YRS)	FY16-25 (10 YRS)
Total DMTS awards	26	23	14	49	74
DMTS with LDRD roots	20	12	14	32	50
% with LDRD roots	77%	52%	100%	65%	74%
Average years from first LDRD experience	16.4	14.5	21.1	15.7	17.7

R&D 100 AWARDS

Another indicator of advancement and leadership in a scientific field is the R&D 100 Awards program, which honors the top innovations of the past year. The renowned R&D 100 competition, now in its 63rd year, received entries from 15 countries and regions around the world. R&D 100 Awards can occur a long time after the initial ideas are developed and after the conclusion of LDRD projects. Typically, it takes 5 to 10 years (or longer) from concept development to receiving an award, including the time needed to move through patenting an invention and demonstrating its commercial applications.

The LDRD program is an investment in our nation's future, ensuring mission support that is often realized many years after an LDRD-funded project concludes.

OVER THE LAST 10 YEARS, 45% OF LLNL'S R&D 100 AWARDS HAD ROOTS IN THE LDRD PROGRAM.

	Single-Year Statistics			Multi-Year Statistics		
	FY23	FY24	FY25	FY16-20 (5 YRS)	FY21-25 (5 YRS)	FY16-25 (10 YRS)
Total R&D 100 Awards	3	3	4	15	16	31
Awards with LDRD roots	2	2	3	4	10	14
% with LDRD roots	100%	67%	75%	27%	63%	45%
Average years from first LDRD experience	14.7	13.5	9	8.8	11.3	10.6

LLNL researchers have won a total of 186 prestigious R&D 100 Awards since 1978.

LLNL SCIENTISTS WIN FOUR 2025 R&D 100 AWARDS; THREE ARE LDRD SUCCESSES

Shown here in the primary mirror surface on a monolithic telescope — one of LLNL's four R&D100 Awards — are reflections of Brian Bauman (left), the space hardware principal optical engineer and inventor of the monolithic telescope, and Frank Ravizza, the space hardware optical engineering lead. (image: Garry McLeod/LLNL)

LLNL scientists and engineers have earned four awards among the top 100 inventions worldwide.

The trade journal *R&D World Magazine* recently announced the winners of the awards, often called the "Oscars of innovation," recognizing new commercial products, technologies and materials that are available for sale or license for their technological significance.

With this year's results, the Laboratory has now collected a total of 186 R&D 100 Awards since 1978. Submitted through LLNL's Innovation and Partnerships Office (IPO), these awards recognize the impact that Livermore innovation, in collaboration with industry partners, can have on the U.S. economy as well as globally.

This year's LLNL R&D 100 Awards include robust telescopes for the environment beyond earth's atmosphere, an x-ray diagnostic for studying rapid phase changes in materials at very high temperature and pressure, a groundbreaking microcapsule production tool and a high-precision additive manufacturing platform for scaled-up production of 3D nano-architectures.

"It's wonderful to see four LLNL teams recognized by the R&D 100 Awards, which highlight the most innovative, game-changing technologies," said Director Budil. "These four projects showcase how we create partnerships — working with industry, government and academia — to create impactful solutions for a wide range of important challenges."

MONOLITHIC TELESCOPES

LLNL's monolithic telescopes address a need for robust, high-performance telescopes in space, an unforgiving environment for instruments onboard space missions. The challenging conditions include high-acceleration launch loads, radiation environments and rapidly varying temperatures from solar exposure.

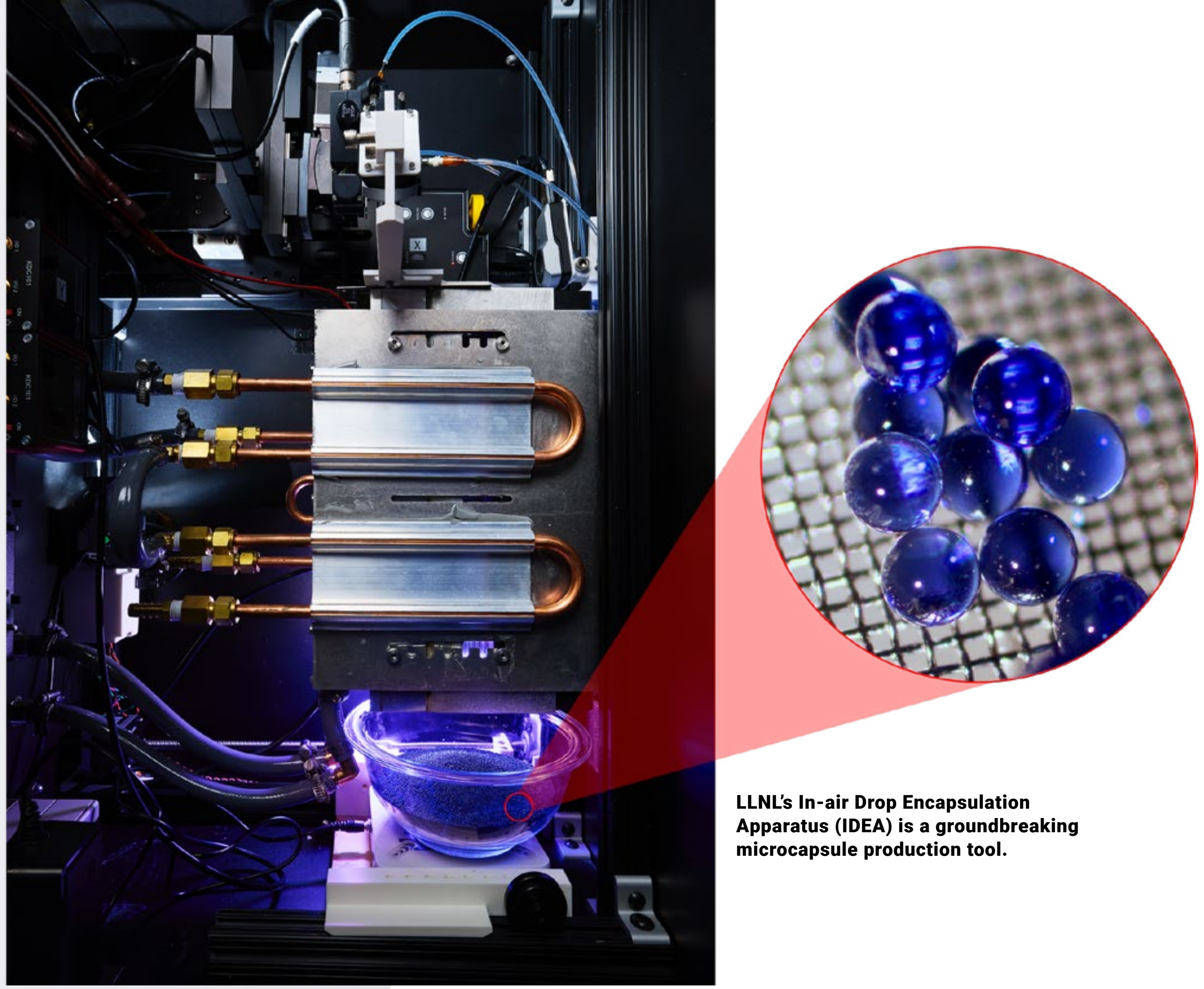
The technology uses monolithic optics, which remain permanently aligned by combining all lens and mirror elements into one solid optic to increase overall mechanical stability and reduce potential points of failure. As the optic is composed of fused silica, its performance is largely unaffected by temperature changes; making it able to endure solar radiation without risking thermal distortions.

Monolithic telescopes offer the functionality of conventional reflective telescopes without the alignment issues that such telescopes face in space environments. And unlike conventional telescopes, the monolithic optic prescription can be tailored to meet a range of mission requirements. For example, infrared and ultraviolet telescopes crafted using this approach can be housed in the same mount design as a visible-band telescope.

Monolithic telescopes have already been flown on demonstration missions with NASA, the U.S. Space Force and commercial partner, Terran Orbital. LLNL is developing monolithic telescopes for upcoming missions in collaborations with Firefly Aerospace and Optimax Space Systems.

Monolithic telescopes were developed by an LLNL team of researchers led by Space Program Leader Ben Bahney, Associate Program Leader for Space Hardware John Ganino and optical engineer Brian Bauman. Principal investigators (PI) also include Frank Ravizza, Willem de Vries, Jordan Smilo, Shawn Higbee and Alex Pertica.

LDRD Project Title:
Monolithic Telescopes
Principal Investigator:
Brian Bauman
LDRD Projects:
10-SI-007,
14-SI-005,
17-ERD-046



LLNL's In-air Drop Encapsulation Apparatus (IDEA) is a groundbreaking microcapsule production tool.

LDRD Project Title:
In-air Drop Encapsulation Apparatus (IDEA)
Principal Investigator:
Congwang Ye
LDRD Project:
18-FS-011

IN-AIR DROP ENCAPSULATION APPARATUS (IDEA)

Microcapsules tailored for maximum effectiveness are in demand for applications like pharmaceutical delivery and sustainable manufacturing. LLNL's In-air Drop Encapsulation Apparatus (IDEA) is a groundbreaking capsule production tool that bridges the gap between industry limitations and application needs.

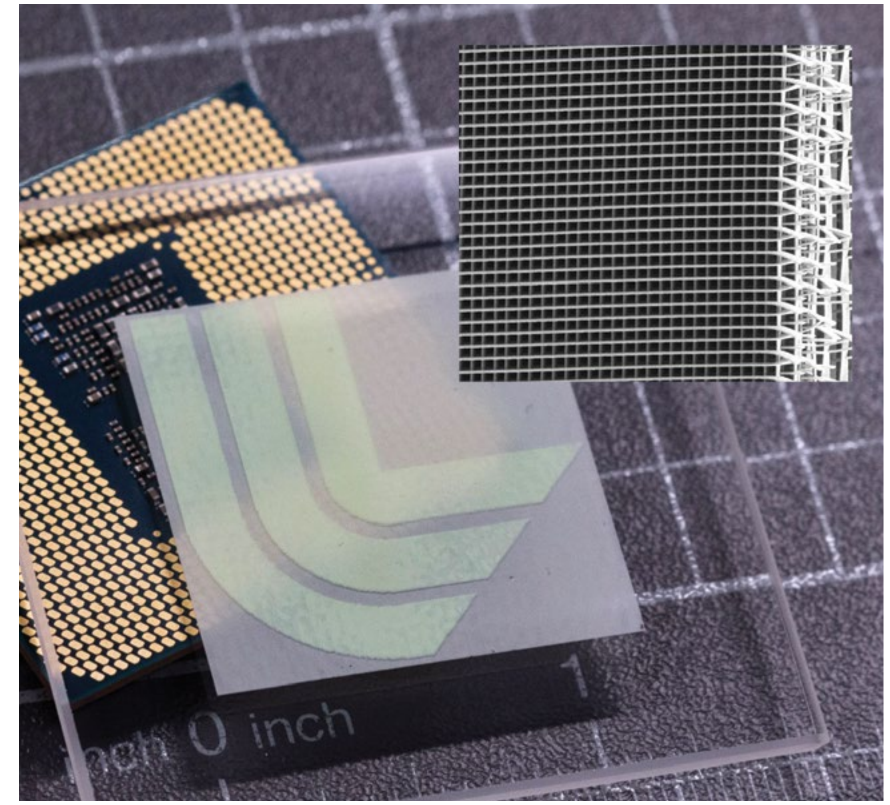
Traditional manufacturing techniques of tailored microcapsules fail to meet yield requirements, create inconsistently sized capsules and waste significant amounts of materials. IDEA offers a scalable solution using diverse, high-performance polymers — enabling encapsulation of reactive or bioactive core solutions at unmatched rates.

Designed to overcome the bottleneck of material availability, IDEA makes lab-developed microcapsules commercially viable. Its success has propelled advancements in bio, energy and many other applications. IDEA is also engineered to significantly minimize waste generation, enhancing the economic and environmental advantages of microencapsulation.

What sets IDEA apart is its ability to produce capsules without relying on a liquid-form continuous phase, while preserving the liquid core essential for modern applications. This unique capability surpasses conventional industrial production techniques, positioning IDEA as a transformative tool in the field.

IDEA was developed by an LLNL team led by PI Congwang Ye and co-developed by Purdue University.

METALITHO3D: METAOPTICS-ENABLED LARGE-SCALE 3D NANOLITHOGRAPHY



MetaLitho3D enables 3D nanolithography at chip scales.

LDRD Project Title:
MetaLitho3D: Metaoptics-enabled Large-scale 3D Nanolithography
Principal Investigator:
XiaoXing Xia
LDRD Projects:
20-FS-032,
22-ERD-004

MetaLitho3D is a one-of-a-kind, high-precision additive manufacturing platform that addresses the limitations of conventional optical systems when scaling up the production rate of 3D nano-architectures to perform wafer-scale, two-photon lithography.

The technology uses over 100,000 high-contrast metalenses and a spatial light modulator to generate a large and tunable focal spot array. This enables the rapid parallel production of complex nano-devices at high resolutions — up to 110 nm, the highest-resolution 3D printing method in existence today. The platform enhances 3D nanofabrication rates by 1,000 times with seamless stitching and a reduction in errors.

MetaLitho3D presents a paradigm shift of 3D nanolithography from laboratory prototyping to wafer-scale manufacturing and fundamentally changes the way 3D nanolithography is performed in current commercial solutions. It enables high-volume production of nanostructures with applications including microelectronics, architected materials, energy, biomedicine and information technologies.

In principle, the fabrication throughput of MetaLitho3D is limitless due to its scaling mechanism, which uses larger metalenses with higher performances. With advancements in supporting technologies such as optical modulators, high-energy lasers and large-scale metalenses, MetaLitho3D could further improve fabrication capacity.

MetaLitho3D team was developed by a team of LLNL researchers led by PIs Xiaoxing Xia and Songyun Gu and co-developed by Stanford University.

Modular Finite Element Methods (MFEM): High-Order Finite Element Algorithms for Next-Generation Exascale Simulations

LLNL's LDRD investments in modular finite element methods (MFEM) have helped transform high-order finite element methods from a specialized research topic into a robust, exascale-ready simulation capability on which multiple mission programs across the Laboratory rely. By consistently focusing on the difficult science: co-designing discretization algorithms, advancing nonconforming adaptive mesh refinement, and delivering performance-portable GPU kernels, the MFEM team has helped maintain the state-of-the-art High-Performance Computing (HPC) used in LLNL's next-generation multi-physics codes. Sharing these advances as open-source software has further amplified the impact of the LDRD investments through broad community adoption and sustained external collaborations. The combination of MFEM's algorithmic innovations, sustained application-driven integration, and maintaining software that scales has allowed the project to have a substantial impact both within the Laboratory and across the scientific computing community.

R&D Challenge

Developing modular finite element methods (MFEM) as a scalable simulation technology that can robustly serve multiple LLNL mission codes required:

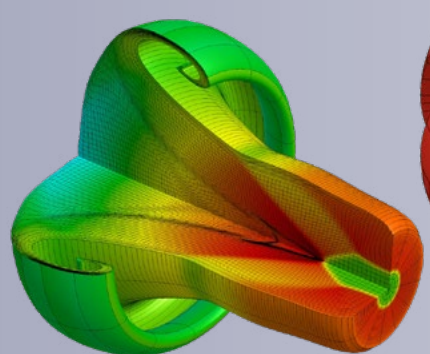
- **Pushing the boundaries of research in HPC and numerical methods for partial differential equations (PDEs).**
- **Sustained close collaboration among researchers in multiple LLNL directorates.**
- **Co-design between algorithm developers and application scientists targeting evolving HPC architectures.**
- **External collaborations facilitated by open-source scientific software.**

Approach

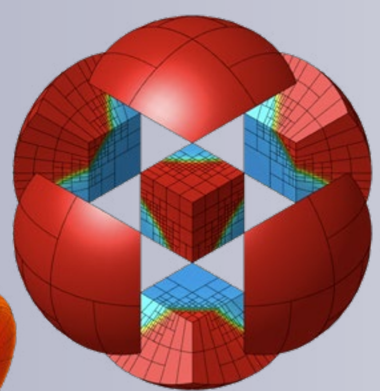
- **Research new high-order finite element algorithms that can both produce better results + scale better on modern systems.**
- **Work closely with scientists in the directorate formerly known as weapons and complex integration, and currently Strategic Deterrence (SD) to demonstrate simulation and HPC benefits on key classes of mission-relevant problems.**
- **Develop state-of-the-art algorithms for high-order meshing, discretizations and solvers driven by application needs.**
- **Advance graphical processing unit (GPU) kernels for performance at scale, developed as part of the effort in the exascale computing project (ECP).**
- **Deliver the R&D into reusable open-source software library to enable modularity and facilitate external collaboration.**

Impact & Benefit

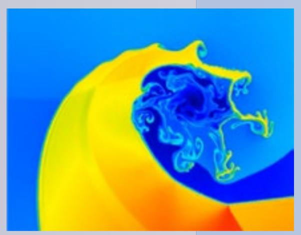
- **Helped establish LLNL as a worldwide leader in finite element research for HPC.**
- **LDRD research resulted in the next-gen BLAST code in SD, enabled other LLNL next-gen efforts, e.g., SMITH and Livermore design optimization (LiDO) in the engineering directorate (ENG).**
- **Broad community adoption (100K+ downloads per year) with many external collaborators.**
- **Supported by advanced simulation and computing (ASC), Office of Science, work for others (WFO), under scientific discovery through advanced computing (SciDAC), Base, high performance computing for manufacturing (HPC4), small business innovation research (SBIR), and Earthshots.**
- **Performed largest finite element simulation to date, 55.5 trillion unknowns on 43,520 GPUs of El Capitan, earning 2025 ACM Gordon Bell Prize.**
- **Continues to drive innovation as a main thrust in the new differentiable multiphysics codes strategic initiative (DMC SI) for differentiable simulations.**



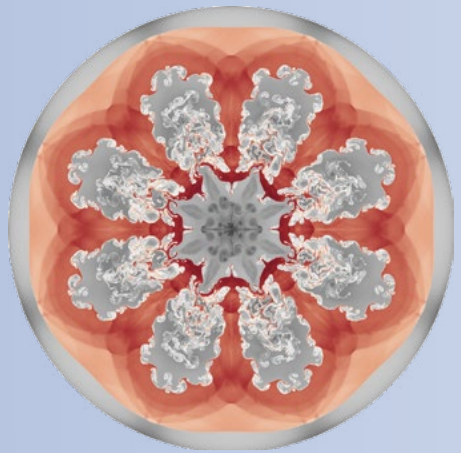
2009 — **LDRD project starts investigating new finite element approaches for Lagrangian Hydrodynamics.**



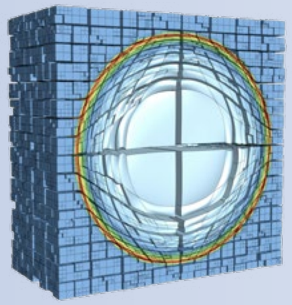
2010 — **Version 1.0 of the MFEM library, developed to aid in the LDRD research, released as open-source.**



2012 — **LDRD builds on MFEM to apply high-order methods to arbitrary Lagrangian-Eulerian (ALE) problems at LLNL.**



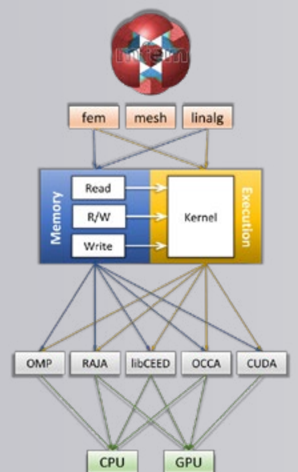
2014 — **Scalable High-Order Computational multi-physics at eXtreme scale (SHOCX) strategic initiative focuses on multi-physics applications. Results in the MFEM-based next-gen BLAST code in WCI/SD.**



2015 — **Added powerful and easy-to-use adaptive mesh refinement capabilities.**

CEED
EXASCALE DISCRETIZATIONS

2017 — **Center for efficient exascale discretizations (CEED) starts developing high-order algorithms for exascale in MFEM.**



2019 — **Initial GPU support added in mfem-4.0.**

2025 — **Gordon Bell Prize for tsunami simulation on El Capitan with MFEM.**

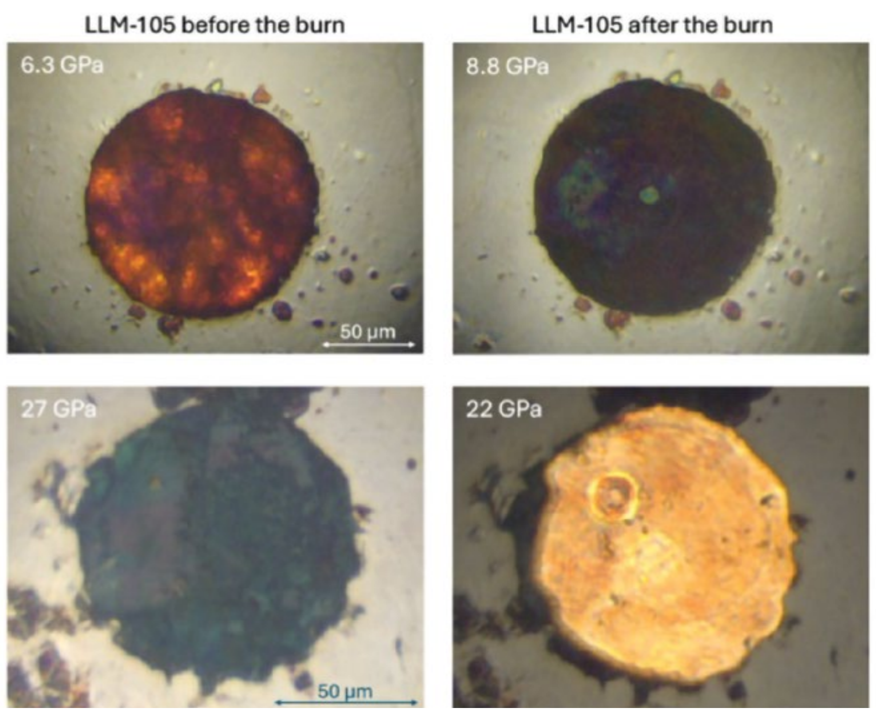
2026 — **Differentiable Multiphysics Codes (DMC) strategic initiative starts to enable differentiable multi-physics codes based on MFEM.**

LDRD-funded research explores the frontiers of science and technology in emerging mission spaces, with projects guided by extremely creative, talented teams of scientists and engineers.

Featured Research

LDRD funded 247 projects in FY25. Here, we provide a closer look at a handful of projects that underscore the exciting, innovative research in this year's LDRD portfolio.

PROBING DEFLAGRATION TO BETTER UNDERSTAND DETONATION



High explosive LLM-105 before and after a laser-initiated burn inside a diamond anvil cell. Sample mass is ~ 1 microgram. The product is opaque at lower pressures and transparent at higher pressures (lower right panel). Note the increase and decrease in pressure, respectively.

Suddenly, there's a flash of intense light and heat, followed by a rapidly expanding fireball. Combustion of high explosives is everywhere in popular culture, and it's also critical for ensuring the safety and reliability of the U.S. stockpile.

While detonations often get all the credit in combustion, deflagrations — their subsonic, less famous precursors — are also fundamental to understanding the safety and sensitivity of high explosives.

In a new study, researchers at LLNL conducted laser ignition experiments in a diamond anvil cell and employed large scale quantum molecular dynamics (QMD) simulations to investigate the products of deflagration at high pressures. The results could improve models of deflagration and high explosives overall.

"A deflagration will generally precede a detonation, so understanding deflagration chemistry is important for understanding the necessary processes that are required for a detonation," said LLNL scientist and first author Brad Steele.

These experiments and models aim to determine the products, or resulting materials, of a deflagration. The composition of deflagration products, especially the solids, influences the amount of energy and pressure released in the reaction and whether it transitions to a detonation.

Typically, deflagration is studied at relatively low pressures. But by using laser ignition in a diamond anvil cell, the team was able to acquire data at high pressures that are comparable to the detonation pressure of high explosive LLM-105.

"The experimental approach is a modernized version of the technique first developed at LLNL in the 1990s," said co-author and project principal investigator Jonathan Crowhurst. "It allows us to probe burn dynamics and chemistry in microscopic samples of high explosives at very high pressures."

At these high pressures, the deflagration products of the experiment were transparent. However, the team's experiment only detected molecular nitrogen, which did not account for the additional elements thought to be present like carbon, hydrogen and oxygen. To better understand this, they looked to simulations.

The researchers used large scale QMD simulations to investigate the pressure dependence of the product chemistry. They found reaction mechanisms that produce extended disordered clusters containing nitrogen and the additional elements.

"The condensed-phase chemistry of energetic materials has typically been simulated using potentials that do not model reaction kinetics accurately. Here we get qualitative agreement with experiment by more accurately modeling reaction kinetics with QMD," said Steele. "The main drawback is that the method is extremely computationally expensive, so it requires the high-performance computing power available here at LLNL."

In both the experiments and models, the authors found evidence of pressure reduction during deflagration. The predicted presence of nitrogen and oxygen in the disordered clusters is consistent with a delay in the formation of gaseous products, a result that could prevent a deflagration from transitioning into a full detonation.

Future work will focus on confirming these findings, applying the techniques to other energetic materials, and incorporating both into practical, macroscopic models that could help guide the design of better high explosives.

Other LLNL authors include Chris Perreault, Jason Baker and Huy Pham.

LDRD Project Title:
Novel Pathways for Storing Energy
Principal Investigator:
Jonathan Crowhurst
LDRD Project:
23-ERD-028
https://doi.org/10.1016/j.combustflame.2025.114067

MAPPING COSMIC SHEAR TO ILLUMINATE DARK ENERGY

This Hubble image features a galaxy cluster that appears to be smiling. The two eyes are elliptical galaxies, while the arcs of the mouth and face are distant galaxies gravitationally lensed by the matter in front of them. While this image shows strong gravitational lensing, the phenomenon also exists on weaker, less noticeable scales. (Image: NASA, ESA, Michael Gladders [University of Chicago], Judy Schmidt)

LDRD Project Title:
Non-Stationary Gaussian Processes at High-Performance Computing Scales for the Space Domain
Principal Investigator:
Amanda Muyskens
LDRD Project:
22-ERD-028
DOI 10.3847/1538-4357/adb0b7

Gravitational lensing often evokes images of a cosmic funhouse mirror: duplicated galaxies, dramatic arcs and distorted shapes. But the web-like, large-scale structure throughout the universe also bends light in a weaker, less obvious way. This phenomenon, known as cosmic shear, can provide clues about the role of dark energy in shaping the universe.

In a recent study published in the *Astrophysical Journal*, researchers from LLNL developed an innovative approach to map cosmic shear using linear algebra, statistics and high-performance computing. With this model, they transformed simulated shear data from specific points into predictions of shear across the sky, effectively filling in observational gaps. The method can handle datasets about 1,000 times larger than previous approaches.

The team focused on quantifying convergence, a measure of how much mass is responsible for lensing at a given location.

"Essentially, our maps create a visual representation of convergence at different points in the window of the sky in which we are looking," said LLNL scientist and author Greg Sallaberry. "If we build these convergence maps at different points in cosmic time [different distances from us], we can start to piece together a history of how structure has evolved across the universe and uncover the role that dark energy plays."

However, creating these maps becomes increasingly computationally challenging as the volume of data grows. With the advent of next-generation wide-field surveys, such as those from the Vera C. Rubin Observatory, researchers will need a scalable method to handle the unprecedented influx of data.

To address this, the team optimized their model by focusing only on nearby data points. Each measurement of convergence was treated as being influenced primarily by its closest neighbors, rather than being tied to every other location in the sky.

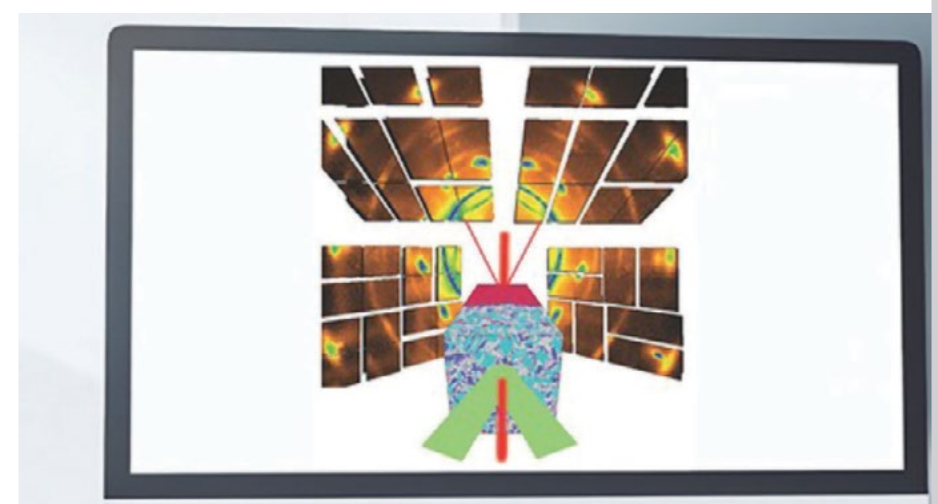
"The computing environment and software stack that makes implementing our model at scale on high-performance computing systems possible was a decade in the making," said LLNL scientist and author Min Priest. "It involves many general-purpose software libraries developed at the Laboratory for large-scale problems."

The study used simplified simulation data, which may not fully reflect the complexities of real-world astronomical surveys. The authors aim to make it more generalizable going forward.

"The endgame is that we want to have a method and associated product that can work out-of-the-box to generate shear maps in a realistic environment," Sallaberry said.

Other LLNL authors include Robert Armstrong, Michael Schneider, Trevor Steil and Keita Iwabuchi. Amanda Muyskens, formerly of LLNL, was chiefly responsible for designing the scalable Gaussian process model.

NEW INSIGHTS INTO METALS UNDER EXTREME CONDITIONS



Femtosecond x-ray snapshot of shock compressed zirconium. (Image: Saransh Soderlind, Patrick Heighway and Raymond Smith/LLNL)

Materials are crucial to modern technology, especially those used in extreme environments like nuclear energy systems and military applications. These materials need to withstand intense pressure, temperature and corrosion. Understanding their lattice-level behavior under such conditions is essential for developing next-generation materials that are more resilient, cheaper, lighter and sustainable.

LLNL scientists and collaborators compressed single crystal samples

LDRD PROGRAM OVERVIEW FY25

of the metal zirconium and found that under high pressure, the material deformed in surprisingly complex ways. The research appears in two journals, *Physical Review Letters* and *Physical Review B*.

Materials under high-stress conditions relieve shear stresses through mechanisms like dislocation slip, crystallographic twinning, shear-induced amorphization, phase transition and fracture.

"Understanding these microscopic mechanisms is vital for developing predictive models of material performance," said LLNL scientist Saransh Soderlind, lead author of this study.

All metals plastically deform — that is, permanently change their shape — under compression primarily due to the motion of defects called dislocations on certain planes in specific crystallographic directions. In the case of zirconium, there is additional complexity due to a change in the crystal structure with pressure.

"The precise knowledge of the crystallographic planes and the direction a material deforms can allow us to develop models describing the mechanical behavior of metals at extreme levels of compression," Soderlind said. "In our work on zirconium, we employed new experimental techniques, which revealed how elemental metals deform in an unexpected and highly complex way."

The team used femtosecond in-situ x-ray diffraction to observe the behavior of single-crystal zirconium compressed to high pressure over nanosecond timescales. The team detected the presence of atomic disorder, a phenomenon never observed in an elemental metal, and discovered multiple pathways for crystal structure transformation, another first-of-its-kind observation.

This disorder and these multiple-phase transition pathways were not observed in polycrystalline zirconium, adding to the novelty of the study. Multi-million atom molecular dynamics simulations using a machine-learned potential corroborated the study's experimental observations.

"These findings reveal a more intricate picture of deformation in metals under extreme conditions than previously understood. This rich tapestry of atomic movements is likely commonplace in other materials at high pressures," said LLNL scientist Raymond Smith, a co-author of this study.

Zirconium alloys are used in the nuclear industry as fuel rod cladding due to zirconium's high strength and low neutron absorption cross-section. It also is extensively used in extreme chemical environments.

Other LLNL contributors include Martin Gorman and Jon Eggert, as well as collaborators from the University of Oxford, AWE and SLAC National Accelerator Laboratory.

LDRD Project Titles: **Kinetics of Incipient Stages of Phase Transitions; Investigating the Relationship between Microstructures and Dynamic Response Using X-Ray Free Electron Lasers**
Principal Investigators: **Raymond Smith, Jon Eggert**
LDRD Projects: **17-ERD-014 and 21-ERD-032**
https://doi.org/10.1103/PhysRevLett.133.096101

ASSESSING ADVERSE NEUROLOGICAL EFFECTS OF WILDFIRE SMOKE INHALATION

Researchers are studying the brain's response to eucalyptus wood smoke extract. Eucalyptus trees are of particular interest due to their high levels of toxicity when burned and their abundance across California, with some reaching between 150–200 feet tall. (Image: Adobe Stock)

Following the devastating fires that swept through Los Angeles in January, 2025, concerns are on the rise about the long-term health impacts of smoke inhalation.

In a study published in the *International Journal of Molecular Sciences*, researchers from LLNL and the Environmental Protection Agency seek to close the knowledge gap on how wildfire smoke exposure can affect the blood–brain barrier, which protects the brain from harmful substances. Such exposure can cause molecular and cellular changes in the brain that are associated with cognitive and neurological dysfunctions, such as Alzheimer's disease, Parkinson's disease and dementia.

While previous studies have mainly focused on understanding the effect of wildfire smoke in the lungs and heart, the latest research has aimed to help identify and understand the potential impacts and adverse outcomes that wildfire smoke exposure can elicit when these particles enter the brain.

The team's study evaluated the responses of two types of in vitro brain cell cultures — brain microvascular endothelial cells (HBMEC) and an immortalized human brain endothelial cell line (hCMEC/D3) — when exposed to varying doses of eucalyptus wood smoke extract over the course of 24 hours.

Eucalyptus trees are of particular interest due to their highly flammable, oil-rich leaves and bark, as well as the high levels of toxicity they release when burned. These factors, combined with their abundance across

California and large size—with some reaching between 150–200 feet tall—pose significant threats to the population.

To the knowledge of the experimental team, this was the first study to investigate the immediate effects of wood smoke extract in brain endothelial cells (which line the blood–brain barrier) using HBMEC and hCMEC/D3.

The research team found that wood smoke exposure induces immune responses in the brain, leading to an increased production of interleukin-8: a cytokine protein, often linked to neuroinflammation, that is released in response to injury or trauma in the body. They also saw evidence of a significant decrease in some of the tight junction markers—a protective component of the blood–brain barrier that seals the space between brain endothelial cells.

Both brain cell types exhibited similar responses to the wood smoke extract, suggesting that either could offer a promising route to study the molecular mechanism of neuroinflammation in the brain from wildfire/wood smoke exposure. The team notes the need for future studies that test longer wood smoke exposure times and analyze other types of brain cells beyond endothelial cells. Taken together, this research may lend new insights into the potential neurotoxicity and crosstalk between the cells.

Additionally, because wildfire smoke particulate matter (fine particles less than 2.5 microns) and volatile combustion products significantly vary in composition depending on the stage of combustion, location, weather, fuel and temperature of the fire, the researchers assert that other types of biomasses beyond smoldering eucalyptus should be assessed to identify which biomass can be more toxic to the brain.

Currently, the LLNL scientists are tracing and quantifying the components of inhaled wildfire smoke in the brain, aiming to identify potential mechanisms of translocation (i.e., the pathway of smoke particles to the brain) using LLNL's Biological Accelerator Mass Spectrometry (bioAMS) capabilities. They also plan to evaluate in vivo neuroinflammatory outcomes of wildfire smoke exposure, which may contribute to neurological dysfunction.

LLNL co-authors of the study include Dorothy You, Bria Gorman, Noah Goshi, Nicholas Hum, Aimy Sebastian, Heather Enright and Bruce Buchholz.

LDRD Project Title:
Adverse Neurological Effects of Wildfire Smoke
Principal Investigator:
Bruce Buchholz
LDRD Project:
23-ERD-020
https://doi.org/10.3390/ijms251910288

LLNL PUSHES FRONTIER OF FUSION TARGET DESIGN WITH AI

Researchers at LLNL have reached a milestone in combining AI with fusion target design by deploying AI agents on powerful supercomputers to accelerate inertial confinement fusion experiments. (Graphic: Dan Herchek/LLNL)

Researchers at LLNL are combining AI with fusion target design by deploying AI agents on two of the world's most powerful supercomputers to automate and accelerate inertial confinement fusion (ICF) experiments.

Part of an AI framework called the Multi-Agent Design Assistant (MADA), LLNL scientists and collaborators are merging large language models (LLMs) with state-of-the-art simulation tools to interpret natural language prompts from human designers and using the platform to generate full physics simulation decks for LLNL's next-generation 3D multiphysics code, MARBL. One of MARBL's key strengths is enabling the design and analysis of mission-relevant, high-energy-density experiments, including ICF.

In ICF experiments at LLNL's National Ignition Facility (NIF), fusion energy is produced when the facility's 192 laser beams converge on a tiny target of deuterium and tritium, creating a fusion chain reaction. The MADA team is using the exascale El Capitan — the world's fastest supercomputer at 2.79 exaFLOPs peak — and its smaller sibling Tuolumne, to test the AI system. The framework incorporates what the team calls an Inverse Design Agent (IDA) to engineer new ICF targets.

Jon Belof, a physicist and principal investigator at LLNL, said the project's origins date back to 2019.

"At the time, we were really interested in the question of what happens if you combine AI with shockwave physics. It was kind of a strange idea — at least a lot of people thought it was," Belof said. "Interestingly enough, that wound up being the simple part. As large language models have advanced, the notion of having semi-autonomous AI systems working alongside the human for ICF design seemed like a natural next step."

But as AI rapidly accelerates in capability and accuracy, the MADA team — which includes National Nuclear Security Administration (NNSA) Tri-Lab collaborators at Los Alamos (LANL) and Sandia National Laboratories — has since turned that "strange idea" into a sophisticated AI-driven design workflow that is getting results.

In a recent demonstration, an open-source LLM — fine-tuned on internal documentation for MARBL — successfully took a hand-drawn capsule diagram and a natural language request from a human designer, then produced a complete simulation deck and ran thousands of simulations to explore variations in ICF capsule geometry to come up with a novel target design.

The AI-driven design paradigm arrives at a critical time for fusion research. Following LLNL's historic ignition achievement at NIF in Dec. 2022, the Laboratory has its sights set on developing a robust ignition platform

LDRD Project Title:
Project DarkStar: Controlling Material Deformation (foundational research)
Principal Investigator:
Jon Belof
LDRD Project:
21-SI-006
https://doi.org/10.1039/D4NR04620J

that would open new possibilities for national security applications.

Belof said tools like MADA — which drastically compresses design cycles and explores vast design spaces — could play a key role in identifying the optimal conditions for scaling up fusion yields. By pairing human insight with AI-driven exploration, LLNL hopes to navigate the complex physics of high-gain implosions faster and more efficiently than ever before.

"In principle, AI agents offer a way for us to pursue not only 3-4 distinct ICF design concepts at once — but hundreds or possibly thousands," Belof explained. "Rather than the human running ensembles of simulations, they will be able to run ensembles of ideas. This concept could be massively transformative in nature."

The heart of the MADA system is its AI "agents" — autonomous software entities composed of two key components: an LLM that can understand and respond to human language, and a specialized "tooling" interface — an executable function that enables the agent to perform domain-specific tasks. For MADA, the agent's tooling can generate structured simulation input files and launch them on HPC systems.

"We are putting AI in the driver's seat of a supercomputer, which is something that has never been done before," Belof said.

Supporting the Inverse Design Agent is another vital component: the Job Management Agent (JMA). While the IDA handles design generation, the JMA drives execution of large-scale simulation workflows across LLNL's supercomputers, interacting with the Flux scheduler and workflow management tools like Merlin.

The JMA ensures jobs are properly queued, resources are allocated, and simulation outputs are efficiently harvested and returned for downstream analysis. Together, these agents operate in a coordinated fashion — the IDA proposing simulation strategies, and the JMA managing the execution pipeline — forming a seamless loop between AI planning and HPC execution.

This iterative workflow enables an unprecedented level of interactivity between designers and their simulations. Instead of manually coding and launching individual jobs — a process that could take days or weeks — researchers can now explore thousands of design variations in parallel, simply by having a conversation with an AI agent.

"The agent can then take a capsule diagram and a plain-language prompt like, 'Explore the effect of changing a certain part of the geometry and translate that into a valid simulation deck for MARBL," Belof explained. "It then runs that deck, collects results, and can even build a training dataset to power a surrogate model."

The MADA approach leveraged HPC to run massive ensembles — typically tens of thousands of ICF simulations in a single study — across LLNL's Tuolumne, the world's 12th fastest supercomputer. The output of these simulations is then used to train a machine-learning model known as PROFESSOR, which can generate instant feedback for designers exploring new capsule geometries.

"Once trained, the PROFESSOR model generates implosion time histories — radius as a function of time — that change instantaneously when the human designer changes the input geometry," Belof said. "It's a powerful new tool to ICF designers that is made possible with AI/machine learning plus HPC."

By enabling natural language interaction, image interpretation and rapid simulation-to-model pipelines, the MADA project demonstrates how AI can be embedded directly into high-stakes scientific workflows. The result is a new stage of national security design work — one that replaces slow, manual iteration with collaborative AI augmentation.

The implications could extend far beyond ICF. As more exascale-class systems like El Capitan come online, MADA offers a blueprint for how AI agents could act as digital collaborators in domains ranging from materials discovery to weapons certification.

"It's really about enhancing human productivity through AI, in a transformative way," Belof said. "And I think this project shows that we're just beginning to tap what's possible. AI tools have the potential for allowing us to best allocate resources and help understand tradeoffs that will be needed for the next generation of enhanced fusion facilities."

NNSA's Advanced Simulation & Computing program is funding the work. Other LLNL MADA team members include deputy principal investigator Charles Jekel, MARBL Project Lead Rob Rieben, and researchers Yue Hao, Kevin Korner, Harshitha Menon, Will Schill, Meir Shachar, Dane Sterbentz and Dan White. Nathan Brown of Sandia and Ismael Djibrilla Boureima of LANL also contributed to the work.

LLNL AND PURDUE UNIVERSITY ACCELERATE DISCOVERY OF MEDICAL COUNTERMEASURES FOR EMERGING CHEMICAL THREATS

From left: chemists Brian Mayer and Katelyn Mason and biologist Todd Corzett observe the operation of the robot that independently executes the acetylchlolinersterase assays the team uses to assess Novichok inhibition and to discover new oxime antidotes for Novichok poisoning. (Photo: Blaise Douros/LLNL)

In a major advance for chemical defense and public safety, scientists at LLNL's Forensic Science Center (FSC) and Purdue University have developed and demonstrated a high-throughput, automated mass spectrometry platform.

Their platform dramatically accelerates the discovery of medical countermeasure candidates against A-series chemical warfare agents, also known as "Novichoks."

The collaborative research, published July 14, 2025, in the *Proceedings of the National Academy of Sciences (PNAS)*, provides the first quantitative data on the potency of these agents and identifies promising new directions for antidote development.

A-series nerve agents have gained notoriety in recent years due to their use in high-profile poisonings. Despite the attention they have received, little experimental data exists about their biological effects or how best to treat exposures.

The LLNL-Purdue team addressed this urgent gap by combining expertise in chemical biology, robotics and advanced mass spectrometry to safely and rapidly conduct thousands of potential antidote reactions — reaching throughput rates of up to 7,000 reactions per hour.

"Rapidly responding to emerging chemical threats like the A-series agents requires new approaches to both understand their dangers and develop effective countermeasures," said Brian Mayer, principal investigator and FSC deputy director.

"By leveraging high-throughput mass spectrometry and automated workflows, we can safely generate the critical data needed to identify promising antidote candidates, even for agents that are closely monitored and extremely hazardous."

The team's enabling technology is an automated, label-free mass spectrometry platform that can analyze complex biochemical reactions in seconds, without the need for traditional markers or dyes. This approach allows researchers to directly measure enzyme inhibition and antidote reactivation in authentic human systems, rather than relying on less-representative animal models or computational predictions.

"This inter-institutional, collaborative model brings the world's best tools to the world's toughest problems — safely and at unprecedented speed," said Graham Cooks, a professor at Purdue University and a co-leader of the study.

The three-year LLNL-Purdue study produced three key findings. First, it provided experimental confirmation that A-series agents inhibit human acetylcholinesterase with potencies similar to traditional nerve agents like sarin and VX. Acetylcholinesterase is an enzyme found in the body, some of which is located in the nervous system, that helps to regulate how nerves talk to each other.

Second, it led to the discovery that certain bispyridinium-based oximes, a class of antidotes, can reactivate enzyme function after A-series exposure — challenging previous reports that these agents are untreatable with existing therapies.

Third, it provided a demonstration of a collaborative, multi-institutional workflow for safely generating nerve agent-adducted enzymes, enabling rapid screening at facilities that cannot directly handle chemical warfare agents.

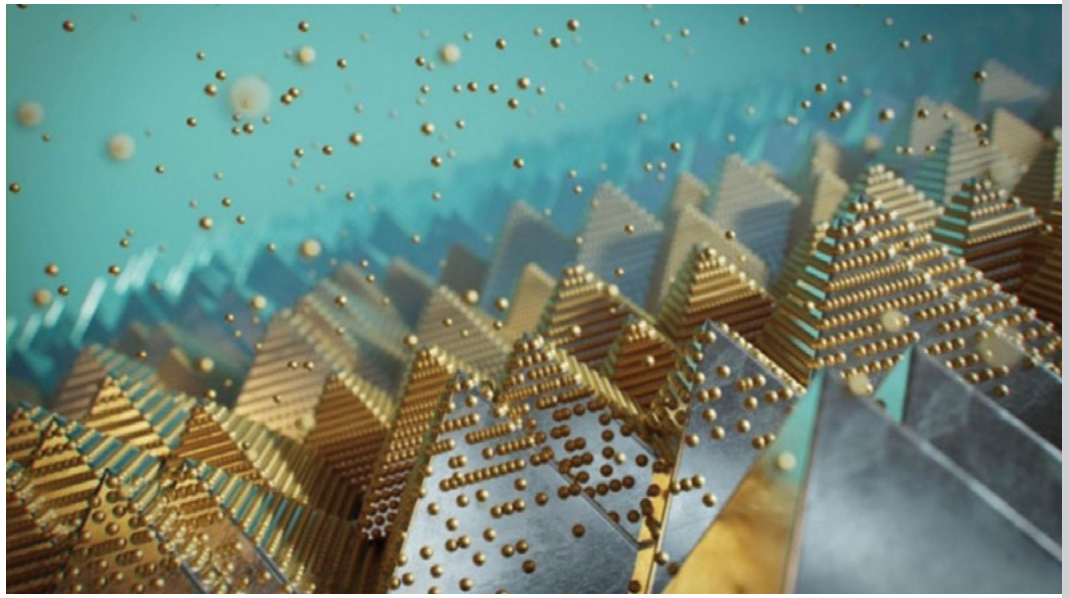
The research underscores the importance of cross-institutional collaboration and technological innovation in national and global security, Mayer said. The automated, joint robotics-mass spectrometry workflow transitioned from Purdue to FSC laboratories not only greatly accelerates the pace of molecular discovery at LLNL, but also dramatically minimizes the risks associated with handling highly toxic substances.

LDRD Project Title:
Countermeasure Development for Chemical-Warfare Agents through Accelerated Molecular Discovery
Principal Investigator:
Brian Mayer
LDRD Project:
22-ERD-007
https://doi.org/10.1073/pnas.2512471122

"This approach allows for rapid, large-scale, safe protein experimentation with authentic chemical warfare agents — something that was previously impractical or impossible," said Audrey Williams, the FSC director. "This capability is essential for staying ahead of emerging threats and ensuring that we have effective medical countermeasures ready when they are needed most."

In addition to Mayer and Cooks, other team members include: Nick Morato, a professor at Purdue University and the paper's first author, and Katelyn Mason, Todd Corzett, Saphon Hok, Teneile Alfaro, Carlos Valdez and all FSC staff members.

DEPOSITING DOTS ON CORRUGATED CHIPS IMPROVES PHOTODETECTOR CAPABILITIES



An illustration of quantum dots as they are deposited on a textured surface. (Image: Brendan Daniel Thompson/LLNL)

Near-infrared photodetectors are used in biomedical sensing and defense and security technologies. For enhanced performance and integrated, compact imaging systems, the photodetectors must be able to detect multiple wavelengths of light at once on a single chip.

Quantum dots, tiny crystals made of semiconducting material, could present a path forward because different-size dots can be engineered to absorb different wavelengths of light. However, depositing films of quantum dots is difficult on the textured, corrugated surfaces used in the infrared regime.

In a study published in ***Nanoscale***, researchers at LLNL presented a new method to deposit quantum-dot films on corrugated surfaces. The technique eliminates the need for post-processing and advances the scalability and performance of quantum dot-based photodetectors.

In the infrared, arrays of pyramids or other microstructures can improve the optical performance of photodetectors by increasing the probability that photons will be absorbed.

"Textured substrates allow for more efficient utilization of incoming infrared light, thereby improving detector responsivity without requiring excessively thick quantum-dot films," said LLNL scientist and author Tom Nakotte. "However, conformally coating such non-planar geometries with uniform, crack-free quantum-dot films is challenging with traditional deposition methods."

To address this problem, the team used electrophoretic deposition, which drives charged particles through a solution with an electric field. When immersed in this liquid environment, quantum dots migrate toward an electrode with the opposite charge. When they reach that electrode, they assemble into a film.

"By turning the electric field on or off, one can start or stop the deposition process," said LLNL scientist and author Christine Orme. "Additionally, since only surfaces under an applied bias receive deposition, electrophoretic deposition naturally enables selective coating — allowing quantum dots to be deposited only on predefined regions of a patterned chip."

Traditionally, quantum dots are synthesized with long organic ligands, molecules that bind to the dots and stabilize them in solution. But after the quantum dots are deposited as a film, those long ligands act as insulators, hinder charge transport, and limit device performance. Removing long ligands with post-processing increases production time and the likelihood of defects, as it can create large cracks in the film.

With careful solvent (liquid) engineering, the researchers fabricated quantum dot films using short ligands, which are more conductive and negate the need for post-processing.

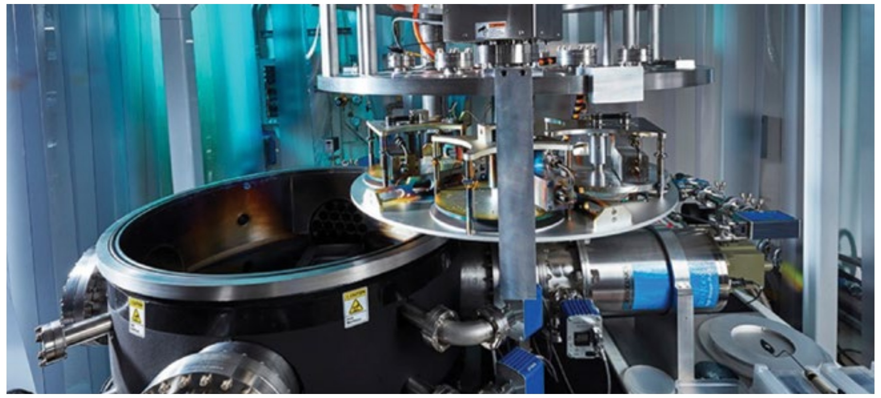
"By combining in-solution ligand exchange with electrophoretic deposition, this paper showed that dense, conformal and electronically functional quantum-dot films can be deposited in a single step," said LLNL scientist and author Xiaojie Xu.

To demonstrate the technique, the group created two simple photoconductors that showed the expected response to light.

While this study demonstrated the ability to create quantum-dot films on patterned substrates, the next step will involve depositing different sizes of the dots on different regions. This will enable tailored sensors that can detect multiple wavelengths of light. LLNL's Jenny Zhou was also an author.

LDRD Project Titles:
Solid-State Gamma-Ray Detection Using Quantum Dots
Principal Investigator:
Tom Nakotte
LDRD Projects:
22-LW-054
https://doi.org/10.1039/D4NR04620J

RESEARCH PROVIDES INSIGHTS INTO ALUMINUM'S OPTICAL PROPERTIES



A magnetron sputtering deposition system at LLNL. Capabilities such as this system allowed researchers to produce the stable, well-characterized aluminum films used in the study.

Aluminum is an important material for a variety of scientific and technological applications, including plasma physics, astrophysics, semiconductor photolithography, and instrumentation for short wavelengths (ultraviolet [UV], extreme ultraviolet [EUV], and x-ray). Despite this common use, and a wealth of experimental data about aluminum, there is still a lack of accurate information about aluminum's optical constants (refractive index), or the properties that determine how aluminum interacts with light. Understanding these properties is important for designing aluminum-based optics and predicting their performance.

In an article published in the *Journal of Applied Physics* and selected as an "Editor's Pick," a team of researchers from LLNL, Université Paris-Saclay, and Lawrence Berkeley National Laboratory describe their work to provide more accurate optical constants for aluminum. Their experiments focused on the EUV and x-ray spectral ranges.

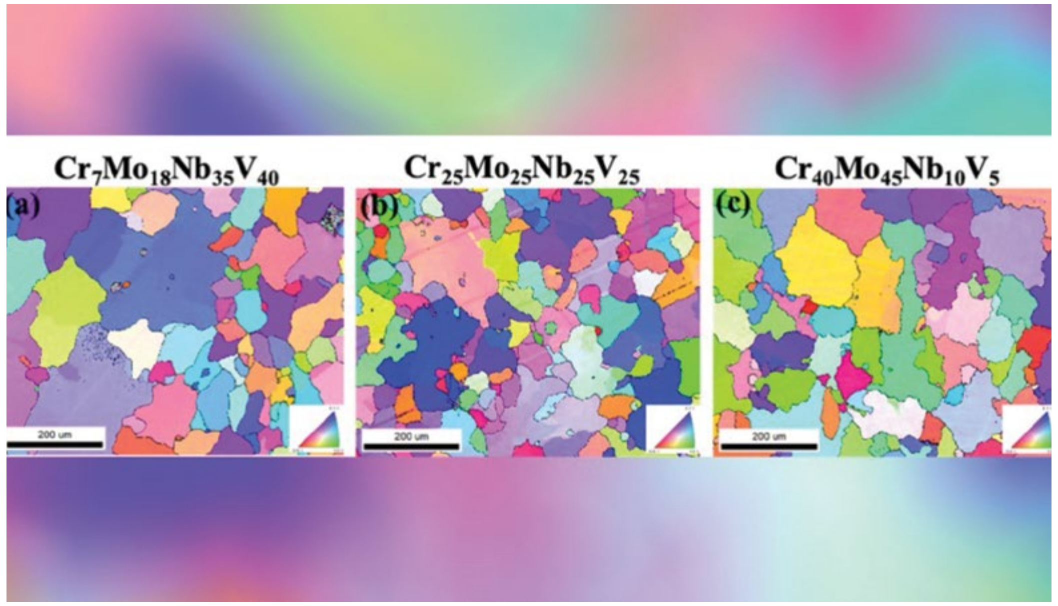
The team constructed freestanding aluminum films with varying thickness, protected by carbon layers to prevent oxidation. Using the Advanced Light Source, they measured the EUV/soft x-ray transmittance (photoabsorption) of each film. They then combined these new measurements with existing data from other spectral regions to calculate how the aluminum dispersed light at different wavelengths.

The result of the team's analysis was a new set of values for the refractive index of aluminum in a wide spectral range, extending from the near-UV to the x-ray region, with ultrahigh resolution near the L absorption edge (L_1 and $L_{2,3}$ regions). The team validated the new optical constants by comparing the experimental results with simulations based on aluminum optical constants from different sources. The agreement between the experimental data and the model using the new optical constants demonstrates increased accuracy compared to models using existing optical constants values from the literature.

The refractive index values from this work support the design, modeling, and calibration of EUV/x-ray instruments. Researchers can also use the values to validate and advance atomic and molecular physics models, such as ab initio calculations.

LDRD Project Title:
Extending the reach of extreme ultraviolet instruments: a new and enabling method for the measurement of the refractive index of materials.
Principal Investigator:
Catherine Burcklen
LDRD Project:
20-FS-026
https://doi.org/10.1063/5.0233781

LLNL'S COMPUTATIONALLY DESIGNED ALLOYS CAPTURE BEST PAPER OF THE YEAR AWARD



Electron back scatter diffraction data shows the grain sizes of the three tested alloys, ranging from 10 to 250 microns.

LLNL researchers have been recognized with the *Journal of Alloys and Compounds*' 2024 best paper award for their publication, "Microstructural, phase, and thermophysical stability of CrMoNbV refractory multi-principal element alloys." The paper examines alloys that have the potential to operate at high temperatures, a feature that enables more efficient engines and mitigates greenhouse gas emission.

"Critical applications in aerospace, energy, and power generation require operating at higher temperatures to achieve higher efficiencies with less fossil fuel," said LLNL researcher and paper author Jibril Shittu. "Ultimately, with improved alloys, we can reduce the carbon footprint of each of these sectors."

Current alloys struggle to withstand temperatures over 1000 degrees Celsius (C) while maintaining their structural integrity. Ceramic materials can handle the heat, but they are brittle and difficult to engineer.

To address these challenges, the team examined refractory multi-principal element alloys, specifically mixtures of chromium, molybdenum, niobium and vanadium. For this class of metals, survivability at high temperatures depends on their microstructural and thermophysical stabilities.

Using LLNL's Materials Acceleration Platform, a computational framework, the scientists narrowed the field of possibilities from 4.6 million to three testable options. They measured mechanical strength and other features of the alloys at a range of high temperatures.

However, testing these properties is not an easy feat. Furnaces and other equipment are mostly developed for superalloys that melt at about 1000–1200 C. This required the authors to redesign and stand up capabilities that were previously nonexistent.

Although one of the alloys showed exceptional strength above 1000 C, another performed even better.

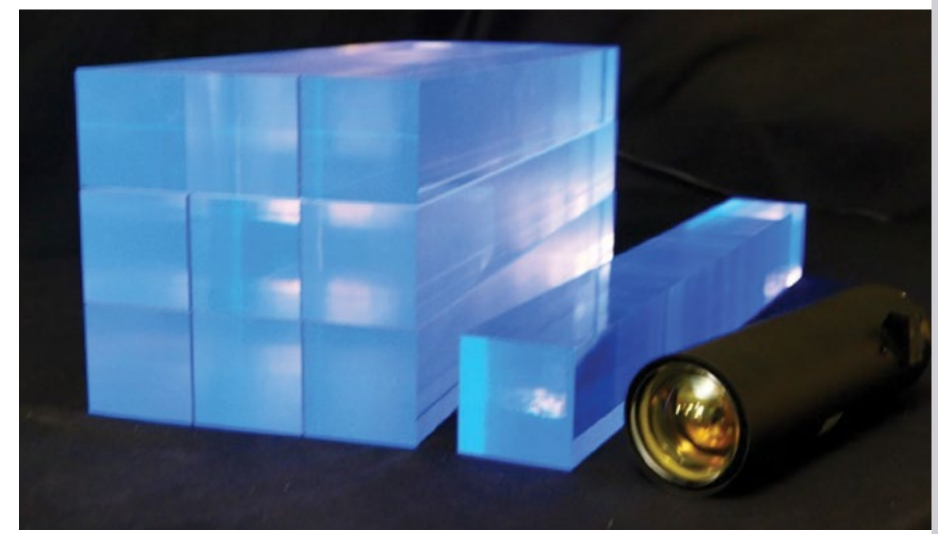
"$Cr_7Mo_{18}Nb_{35}V_{40}$ maintains microstructural, phase, and thermophysical stability at all relevant operating temperatures needed to satisfy high-temperature stability and survivability," said Shittu. "This result highlights the need for high-temperature stability and survivability of alloys over exceptional strength as a design criterion."

This award-winning publication demonstrates that LLNL's computational framework can be used to identify viable new alloys for any tailored application. Such a capability cuts alloy discovery and validation time from years to months.

"The strength of our science at LLNL lies in collaboration, by pooling diverse skill sets and perspectives," said Shittu. "Making a significant research impact of this nature can only be realized by bringing the unique experience and expertise of every team member to the table for a comprehensive and well-rounded solution. This success is truly a team effort."

LDRD Project Title:
Rapid Design to Deployment of Tailored Alloys
Principal Investigator:
Joseph McKeown
LDRD Project:
22-SI-007
https://doi.org/10.1016/j.jallcom.2023.173349

"LIGHTING" UP ANTINEUTRINO DETECTION



Building on more than a decade of research, LLNL materials scientists and industry partner Eljen Technology have produced plastic, lithium-6 doped scintillator "bars" (with dimensions of 5.5 cm × 5.5 cm × 50 cm) capable of detecting antineutrinos: the antimatter partner of a neutrino, one of nature's most elusive and least understood subatomic particles.

How do you find and measure nuclear particles, like antineutrinos, that travel near the speed of light?

Antineutrinos are the antimatter partner of a neutrino, one of nature's most elusive and least understood subatomic particles. They are commonly observed near nuclear reactors, which emit copious amounts of antineutrinos, but they also are found abundantly throughout the universe as a result of Earth's natural radioactivity, with most of them originating from the decay of potassium-40, thorium-232 and uranium-238 isotopes.

When an antineutrino collides with a proton, a positron and a neutron are produced — a process known as inverse beta decay (IBD). This event causes scintillating materials to light up, making it possible to detect these antineutrinos; and if they can be detected, they can be used to study the properties of a reactor's core or Earth's interior.

Researchers at LLNL, in partnership with Eljen Technology, are working on one possible detection solution — a plastic, lithium-6 doped scintillator for detecting reactor antineutrinos that represents over a decade of materials science research. Their research appears in the journal of *Nuclear Instruments and Methods in Physics Research Section A.*

MAGIC IN PLASTIC

In the early 2010s, LLNL materials scientist Natalia Zaitseva and her team were the first to develop a plastic scintillator capable of pulse-shape discrimination (PSD), i.e., efficiently distinguishing neutrons from gamma rays (important for detecting IBD events). Building upon this work, the new lithium-6-doped plastic scintillator formulation also is PSD-capable.

"Lithium-6 is particularly advantageous because, in addition to having a significant thermal-neutron-capture cross section, it offers a localized capture location, further enhancing the detector's ability to effectively reject unwanted background noise," said LLNL scientist Viacheslav "Slava" Li. This enhanced detection is made possible through the IBD process.

"While integrating lithium-6 into liquid scintillators has proven to be a challenging yet rewarding endeavor—successfully demonstrated by PROSPECT, another reactor-antineutrino experiment with fundamental LLNL contributions — achieving this in a solid, compact and easily transportable plastic scintillator has not been accomplished before, especially not at a scale suitable for effective antineutrino detection," said Cristian Roca, LLNL scientist and corresponding author of the paper.

Compared to liquid scintillators, which have been the standard technology for reactor–antineutrino detection for decades, plastic scintillators offer superior safety and mobility with fewer of the regulatory and practicality constraints that are typically placed upon liquid scintillators and their operating environment.

LDRD Project Title:
The Next Frontiers in Rare Event Detection for Science and Security
Principal Investigator:
Nathanial Bowden
LDRD Project:
20-SI-003
https://doi.org/10.1103/PhysRevApplied.22.054030

OPTIMIZING DETECTOR PERFORMANCE

To ready the scintillator (commercially known as EJ-299-50) for the market, researchers in LLNL's Rare Event Detection group conducted a series of characterization measurements of the material's performance in a large-scale detector system. The team's research was funded by LLNL's Laboratory Directed Research and Development program and the National Nuclear Security Administration's Office of Defense Nuclear Nonproliferation Mobile Antineutrino Demonstrator project.

For almost six months, researchers studied the aging process of these scintillators to ensure the long-term stability of the plastic. After demonstrating the reliable optical performance and neutron identification capabilities of EJ-299-50 during this time, researchers installed 36 of the plastic scintillator "bars" in a 6 × 6 grid configuration on a detection system called the Reactor Operations Antineutrino Detection Surface Testbed Rover (ROADSTR). A follow-on study is currently underway to evaluate ROADSTR's performance with these bars.

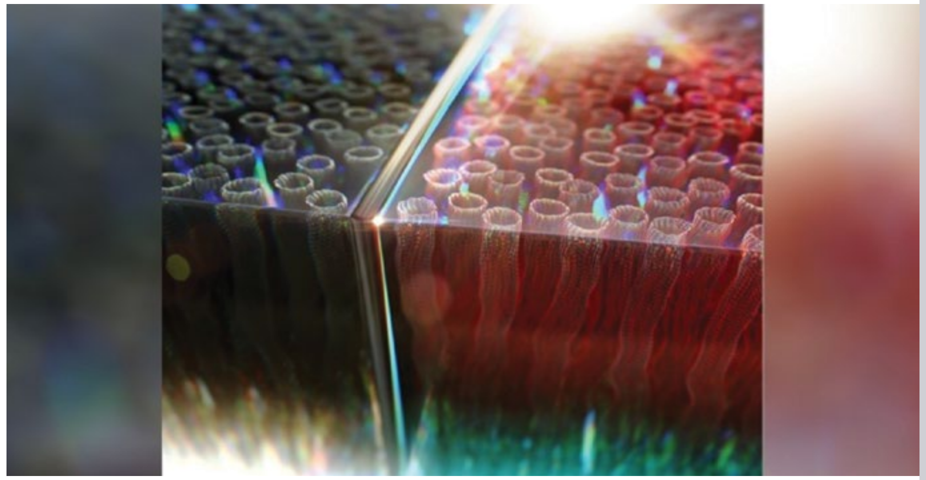
Alongside their scintillator work, scientists in the Rare Event Detection group are collaborating with researchers at the University of Hawai'i to improve the directional sensitivity of detectors; i.e., the ability to determine the direction of the incoming antineutrino in relation to the detector. This information can be extracted by correlating the events that take place during the IBD reaction and is especially useful in constraining the illicit production of weapons material.

The team's research, published in *Physical Review Applied* and supported by the Consortium for Monitoring, Technology and Verification, explores different detector designs, finding that certain detector geometries outperform others in terms of directional resolution.

With applications in reactor safeguards and monitoring, as well as homeland security and nuclear non-proliferation, these combined research efforts are opening the door to a new era of antineutrino detection.

In addition to Zaitseva, Li and Roca, LLNL co-authors of these studies include Nathaniel Bowden, Leslie Carman, Steven Dazeley, Sean Durham, Michael Ford, Andrew Glenn, Michael Mendenhall, Felicia Sutanto and Marc Bergevin.

CARBON NANOTUBE "SMART WINDOWS" OFFER ENERGY SAVINGS



LLNL researchers have developed "smart" windows with vertically aligned carbon nanotubes that can modulate the transmission of near-infrared light, potentially cutting costs and energy usage in modern infrastructure. (Image: Jeremy Gardner/LLNL)

Half of the sun's radiant energy falls outside of the visible spectrum. On a cold day, this extra infrared light provides additional warmth to residential and commercial buildings. On a warm day, it leads to unwanted heating that must be dealt with through energy-intensive climate control methods such as air-conditioning.

Visibly transparent "smart windows" that can modulate the transmission of near infrared light offer one potential cost- and energy-saving measure for modern infrastructure.

To work towards solving this technological challenge, a multidisciplinary team of researchers at LLNL developed a new type of electrically controlled, near-infrared smart window that can cut near-infrared light transmission by almost 50%. Their secret ingredient? Vertically aligned carbon nanotubes — tiny, tube-shaped structures made from carbon atoms that are thousands of times thinner than a human hair. The research was published in *Nano Letters*.

In these smart windows, the carbon nanotubes are grown so they stand upright on the glass, like a microscopic forest. Because these current devices are just millimeters in size, the team noted that scaling-up the technology will be a necessary next step.

Depending on the voltage applied, the nanotubes can either absorb infrared light and block heat from the sun or let the infrared light through. One critical feature of this technology is that once they are put into either a blocking or transparent state, the carbon nanotubes retain charge well, like a battery, and so a continuous voltage is not needed to maintain that state. This offers extremely low-power operation, a necessity to drive energy savings for the end user.

To come up with this design, the researchers coupled experimental fabrication and measurements from modeling efforts to better understand the microscopic physics that drive the tunable infrared response, yielding new insights into the optical and electronic physics of vertically aligned carbon nanotubes.

Their work builds on nearly a decade of LLNL research into the synthesis and study of vertically aligned carbon nanotubes.

LDRD Project Title:
Materials for Energy Management Across the Electromagnetic Spectrum
Principal Investigator:
Anna Hiszpanski
LDRD Project:
23-ERD-049
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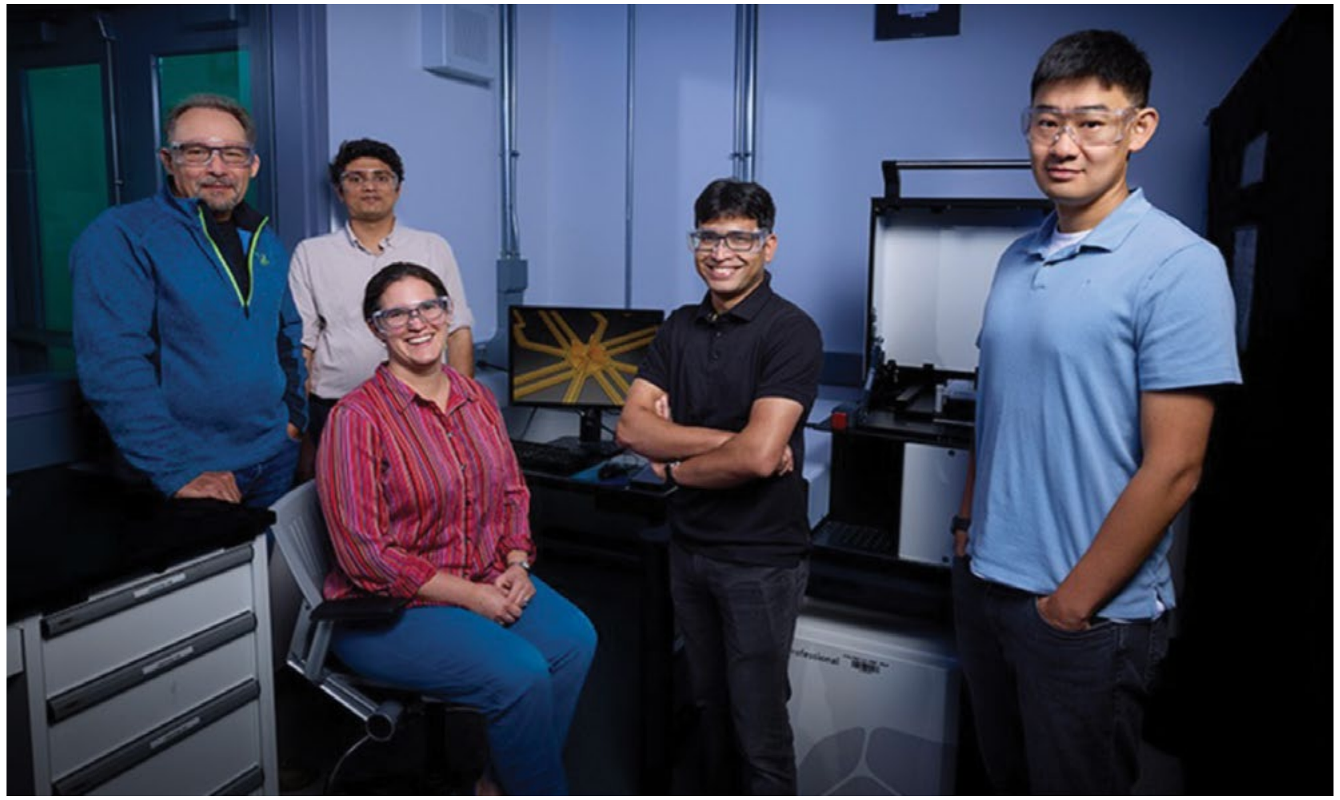
MINIATURIZED ION TRAPS SHOW PROMISE OF 3D PRINTING FOR QUANTUM-COMPUTING HARDWARE



From left: Lawrence Livermore National Laboratory Materials Science Division (MSD) researcher Juergen Biener, Materials Engineering Division(MED) staff engineer Abhinav Parakh, physicist Kristin Beck, physics postdoctoral researcher Sayan Patra, and MED staff engineer Xiaoxing Xia. (Photo: Garry McLeod/LLNL)

Researchers at LLNL, the University of California (UC) Berkeley, UC Riverside and UC Santa Barbara have miniaturized quadrupole ion traps for the first time with 3D printing — a breakthrough in one of the most promising approaches to building a large-scale quantum computer.

Quadrupole ion traps have four electrode poles that create an oscillating electrical potential that traps ions by overriding their natural vibration, similar to how raising or lowering different ends of a playground parachute can keep a soccer ball on its surface. The traps keep ions confined for hours before they escape, and if the ions are cooled to their ground state — where they are at their lowest possible energy — they can function as quantum bits (qubits), the most basic unit of information in a quantum computer.

Made with ultrahigh-resolution, two-photon polymerization (2PP) 3D printing, the millimeter-scale ion traps can confine calcium ions with frequencies, error rates and coherence competitive with the state-of-the-art and can be used to perform single- and two-qubit operations. The team's findings were published in a recent paper in *Nature*.

"This is the sort of technological change that's going to take ion traps from working well with just a few ions to doing something that we would consider a computation and, hopefully, to something we can start using as a computer," said co-author Kristi Beck, LLNL physicist and director of the Livermore Center for Quantum Science. Qubits need to remain coherent (in a quantum state) for as long as possible and behave as reliably as possible for researchers to effectively encode data and perform operations. Trapped ions have much longer coherence times and work at higher temperatures than other approaches — requiring a laser to cool ions to their ground state instead of cryogenic refrigeration. However, there is a tradeoff between performance and scalability. In industry, researchers commonly use "planar" ion traps with surface electrodes that can scale well as building blocks of a large-scale information processing system, but the traditional 3D designs have better performance.

The team saw a potential solution to this problem in 3D printing."3D printing gives us the confinement we need to trap the ion well and at high frequencies, and we can also make many ion traps on the same chip," said Materials Engineering Division (MED) staff engineer and co-first author Xiaoxing Xia. "This is similar to when people worked with bulky, individual transistors before the integrated circuit was invented. 3D printing can allow us to move beyond these conventional traps into more highly integrated systems like our current processors."

The printed traps can confine calcium ions with much higher frequencies than both the regular 3D traps and planar traps, creating deep harmonic potentials between electrodes that stabilize the system and improve coherence. The traps demonstrated their stability by confining two calcium ions that exchanged positions every few minutes — competitive with the state-of-the-art.

The team also implemented a two-qubit entangling gate with 98% fidelity, performed single qubit rotations and measured motional heating rates, which quantify one of the primary sources of error for trapped ion quantum gates.

"I'm excited by the potential that opens up from just our proof of concept," said MED staff engineer and co-author Abhinav Parakh. "To be able to harness the exponential computational power [from quantum computing], we need to have multiple ions entangled with each other, bring them close, do computation with them, and then pull them apart — something can be done efficiently using 3D printed structures."

The team can reliably print a miniaturized ion trap in 14 hours from scratch, or in 30 minutes if they only print the electrodes on an existing substrate. The ability to rapidly prototype and the flexibility to print in nearly any configuration also gives them a chance to experiment with new designs, such as a planar trap based on the classic 3D design that the team developed, printed, miniaturized and used to trap ions at both cryogenic and room temperatures.

"As designs evolve, the team aims to integrate photonics and electronics on the same chip to make the entire system more efficient and compact. Beck also wants to explore ways to make quantum computers more reliable and easier to control. The greatest source of error is noise, uncontrolled interactions with the environment that make a quantum system behave unreliably, and the surfaces of ion traps are currently a major source of noise.

"If we can take away more material that is close to the ions, there's going to be fewer places where we know that noise is entering into the system, so we expect to see better performance," she said.

A POTENTIAL CATALYST

The project was originally supported by a UC National Laboratory Fees Research Program, which fostered the collaboration among LLNL, UC Berkeley, UC Riverside and UC Santa Barbara.

"By reinvesting and continually refining how we direct the fees earned from managing our national labs, the University of California is proud to support high-impact collaborations by bringing together talent and expertise that open doors to breakthrough science and speed discoveries," said June Yu, vice president of UC National Laboratories.

Materials Science Division (MSD) researcher Juergen Biener, who was co-PI on the project with Haeffner, credits the project's success to this partnership.

"Getting this world-class expertise together to share ideas and work as a team is the type of thing that really accelerates a field," Biener said. "Within three years, we went from zero to almost state-of-the-art in a fairly competitive field and I think that, in itself, tells a story."

The team hopes their innovative approach will help put LLNL on the map for ion trap quantum computing hardware development and serve as a potential catalyst for future collaborations that will help transform their ideas into commercial products.

The miniaturized ion traps can also be used for sensing and ultra-precise atomic clocks, and if the laser cooling system is successfully scaled and integrated on a chip, they could be the basis for compact, low-power mass spectrometers for precision metrology. Xia also sees it as an opportunity to show what high-resolution 3D printing can do for the field.

"Quantum computing is an ideal early adopter for 3D printing because they want the very high resolution, fine features and intricate 3D geometry that no other fabrication technique can provide," said Xia.

Other co-authors on the paper include Shuqi Xu, Qian Yu, Sumanta Khan, Eli Megidish, and Bingran You from UC Berkeley, Boerge Hemmerling from UC Riverside, and Andrew Jayich from UC Santa Barbara.

LDRD Project Title:
Three-Dimensional Ion Traps to Enable Quantum Error Correctable and Scalable Quantum Computing
Principal Investigator:
Kristin Beck
LDRD Project Number:
23-ERD-021
https://doi.org/10.1038/s41586-025-09474-1

LDRD/SDRD Interlaboratory Pilot Program

UNLEASHING OUR NATION'S POTENTIAL THROUGH INTERLABORATORY COLLABORATIONS

There is a long history of formal and informal collaboration between the Department of Energy National Laboratories and sites. Institutions invest in these collaborations because of shared goals and because experience has shown that the combined strengths and capabilities of multiple institutions can be a force multiplier in achieving impactful outcomes for the nation. Interlaboratory (IL) projects are intended to leverage the unique capabilities of each collaborating laboratory or site to produce transformational outcomes that exceed what could be achieved by a single institution and will thereby strengthen mission impact. Teams are drawn from institutions participating in the IL call. Laboratory Directed Research and Development (LDRD) and Site Directed Research and Development (SDRD) IL projects must create new collaborations, either (a) from teams that have not worked together or (b) through the addition of new team members to established collaborations.

IL LDRD/SDRD PILOT PROGRAM FAST FACTS

In July of 2023, the first call for IL proposals was issued with three laboratories participating: Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Sandia National Laboratories (Sandia). A total of 125 Letters of Intent (LOIs) were received, and 79 invited full proposals were submitted. Six projects were selected from that initial call.

Based on the enthusiasm of the first call, a second proposal call was announced in July of 2024. Laboratory participation in the call increased with the addition of Idaho National Laboratory (INL), Nevada National Security Sites (NNSS), and Pacific Northwest National Laboratory (PNNL).

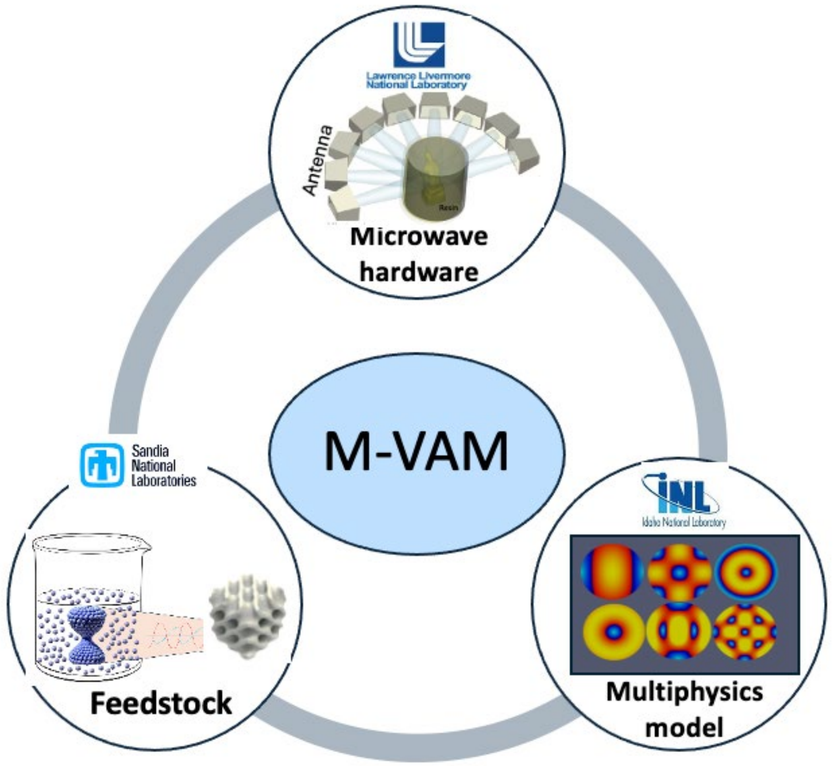
Multi-lab teams submitted proposals to one of four focus areas: advanced manufacturing, fundamental AI for science, energy security, and radiographic systems.

The response to the call was robust; a total of 127 LOIs were received and 25 invited full proposals were submitted. Seven 3-year projects were selected through a rigorous, multi-institutional committee review process.

Funding for the seven projects was issued to the principal investigators (PI) at the beginning of 2025. We are excited to share with you highlights and details from each of the four LLNL projects that were selected for funding through the July 2024 proposal call. These collaborative projects started in January of 2025 and will continue through September of 2027.

RAPID, SCALABLE 3-DIMENSIONAL CERAMIC FABRICATION VIA MICROWAVE-ASSISTED VOLUMETRIC ADDITIVE MANUFACTURING

LLNL PI: SAPTARSHI MUKHERJEE
SANDIA PI: KEVIN STRONG
INL PI: DONNA POST GUILLEN



This project is developing an energy efficient, fast, and scalable microwave volumetric additive manufacturing (M-VAM) system that combines innovations in ceramic processing, microwave beamforming and multiphysics modeling. M-VAM enables a game-changing AM technology capable of rapidly printing large volumes (~1 ft distance, time <1 hour) of opaque materials, currently not accessible by conventional AM approaches. This revolutionary approach will unlock important applications such as developing extreme environment and high-toughness materials, impacting multiple DOE mission areas, especially nuclear power.

The team's experimental beamforming system employs multiple antennae to enable volumetric printing for opaque ceramic materials, marking significant progress. This innovative approach contrasts with current stereolithography techniques that require large volumes of polymer binders, resulting in processing defects (e.g., voids, debinding and/or delamination cracks) and extended processing times. Instead, the use of microwave absorptive polymers in low volume fractions allows for rapid curing of green bodies. Additionally, a technique to locally gel colloidal particles through aggregation mechanisms to form a 3D body is being investigated. Temperature controlled solubility properties of organogelator chemistries will enable thermally controlled gelation of fluid phase. A high-fidelity 3D Multiphysics Object-Oriented Simulation Environment (MOOSE) model integrates microwave thermal diffusion with colloidal ceramic curing kinetics to optimize resolution, processing parameters, and scalability.

This advanced microwave M-VAM system enables large-scale ceramic printed parts and offers predictive capabilities to guide efficient resource utilization and facilitate scaling from laboratory to industrial scale. The multiphysics modeling approach is a powerful tool poised to significantly advance the scalability of ceramic AM technologies. Additionally, a unique pulsed hardware is being developed that can shape tailored nanosecond pulse bursts to enable high resolution in M-VAM.

WHAT THE TEAM IS SAYING

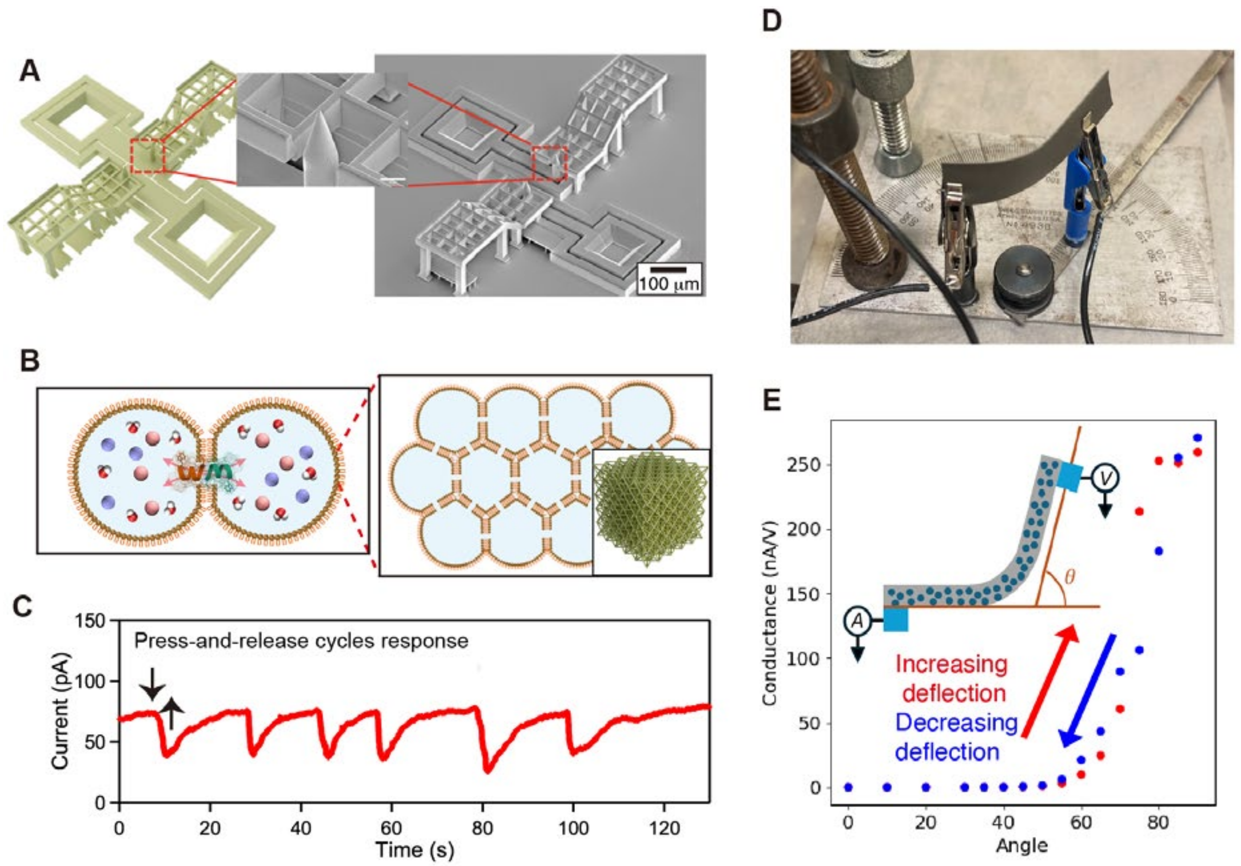
"Harnessing the collective expertise of researchers across DOE laboratories allows us to synergize experimental efforts with advanced computational modeling, propelling this advanced manufacturing technology towards success." – **Donna Post Guillen, INL**

"M-VAM opens up a new frontier in large-scale 3D printing with enhanced material properties by enabling the use of opaque materials, which had previously posed challenges in additive manufacturing processes. Each DOE laboratory brings its unique expertise to solve this exciting, multi-disciplinary problem and expand the definition of 'what's printable'."– **Saptarshi Mukherjee, LLNL**

"Leveraging Sandia's expertise in ceramic processing alongside Lawrence Livermore's innovations in microwave forming, and harnessing Idaho's computational prowess, this collaborative project represents a groundbreaking convergence of disciplines. Together, we are poised to transform advanced manufacturing techniques and bring this innovative approach to fruition."– **Kevin Strong, Sandia**

ADDITIVELY-MANUFACTURED SELF-REPORTING NEUROMORPHIC SMART MATERIALS FOR AUTONOMOUS SENSING AND COMPUTING

LLNL PI: ALEKSANDR NOY
SANDIA PI: ALEC TALIN



A. Schematics and an SEM image of a 3D-printed scaffold for forming individual droplet interfaces. Inset highlights the 3D-printed needle electrode.
B. Schematics of the droplet-interface-bilayer (DIB) emulsion-based smart solid. Inset shows a 3D-printed flexible scaffold that we integrate with the emulsion.
C. Preliminary data mapping ionic current response of the DIB emulsion slab to several cycles of applied pressure.
D,E. Testing setup (D) and conductance vs bending angle data (E) showing large, reversible and reproducible change in conductance of a custom metal/silicone during mechanical deformation.

The goal of this project is to develop materials with a microstructure that enables objects made from these materials to sense their shape as well as vibrations, temperature, and potentially other aspects of their environment. These "smart" materials are based on a distributed artificial neural network of shape-sensing memory elements embedded in additively manufactured scaffolds which reports its topology, shape and dynamic changes in response to applied strain. Our approach is to demonstrate this concept in a series of assemblies and materials starting with simple networks comprising a handful of synaptic elements that detect and process basic changes in shape (e.g., bending) to larger distributed reservoirs embedded in 3D-printed scaffolds to detect and process complex changes object geometry. These materials will enable a new generation of applications that combine sophisticated sensing and information processing capabilities for monitoring of structural integrity and damage for applications such as accident response hardware, deformation dynamics in critical loadbearing structures, enhanced situational awareness for autonomous underwater vehicles, and other national security applications of mutual interest to DOE labs.

In the first several months of this IL collaboration, the team at LLNL has developed scaffolds for assembling and testing synaptic junction primitives (Figure 1A) and is currently testing their response. LLNL team has already assembled droplets emulsions that exhibit reservoir response, integrated them with 3D printed elastic scaffolds, and showed that they can dynamically respond to applied pressure using testing hardware and protocols developed by the Sandia team (Figure 1C,D). To validate this approach with a distinct class of materials, Sandia and LLNL team members have also demonstrated the ability to sense and process shape changes using polymer-dispersed metallic particles (Figure 1D,E).

This IL-LDRD funding has been a very strong effort multiplier that has allowed the laboratory teams to make significant progress during the first few months of the project. Every project that brings together teams with different technical expertise, skills, and approaches involves a learning curve, and this project is no exception. The LLNL team has a lot to learn from the Sandia team engineering prowess, their deep expertise in neuromorphic device architecture, design, and testing. LLNL's materials and manufacturing expertise helped Sandia's team design the testing hardware and protocols. The combined multi-lab team is looking forward to the next steps in this IL-LDRD project that leveraged unique expertise of different NNSA laboratories to push the boundaries of smart materials design for national security applications.

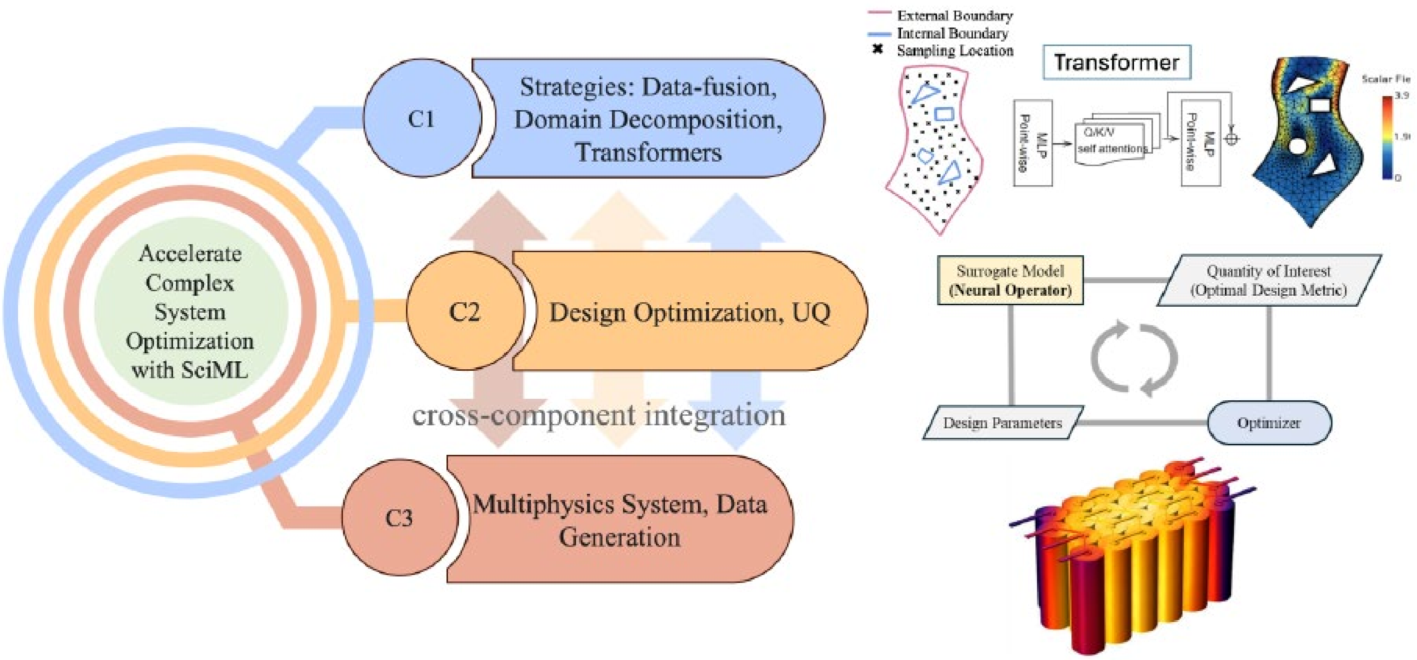
WHAT THE TEAM IS SAYING

"Sometimes quantity does translate into quality. I am amazed every day how this quickly this collaboration can proceed when we combine the expertise of several different national laboratory teams. This is truly an interdisciplinary team effort that represents the type of research project that national laboratories do best." – **Alex Noy, LLNL**

"We have a highly collaborative team with complementary capabilities focused on a common goal to solve tough problems through innovation and trust" – **Alec Talin, Sandia**

DATA-FUSION WITH PHYSICS-INFORMED NEURAL OPERATORS FOR FAST AND ROBUST PREDICTION OF MULTIPHYSICS SYSTEMS AS DESIGN SURROGATES

LLNL PI: PRATANU ROY
PNNL PI: YUCHENG FU
SANDIA PI: MICHAEL PENWARDEN



Structure of the research scope, showcasing the division of research into three main components.

This project aims to advance neural operators through physics-informed methodologies within scientific machine learning (SciML) to develop fast, accurate, and generalizable surrogate models for multidisciplinary applications. These applications include design optimization in energy storage, subsurface transport, and multi-material moisture sorption — domains where computationally expensive simulations often limit progress. By addressing the key challenge of integrating multi-fidelity data into SciML frameworks, this collaboration leverages experimental and numerical datasets of varying fidelity and uncertainty alongside physics-informed governing equations. The objective is to create neural operator models that seamlessly fuse diverse data sources while quantifying uncertainties tied to inputs. These models will significantly reduce computational costs, enable rapid optimization, and enhance extrapolation and generalization across complex multiphysics systems. Through the combined expertise of LLNL, Sandia, and PNNL, this effort lays the groundwork for advancing artificial intelligence (AI) and machine learning (ML) technologies to solve critical scientific and engineering challenges.

At the starting stage of this project, the team has established an efficient framework for interlaboratory collaboration by aligning the project's tasks with the expertise of individual researchers across three labs, in addition to more frequent focus area meetings. To maintain efficiency and alignment, the team conducts monthly roundtable updates where each focus area presents concise one-slide summaries of progress, challenges, and planned next steps to promotes transparency, facilitates knowledge exchange, and keeps all partners informed of key milestones and shared goals.

The generation of multi-fidelity datasets for multiphysics systems is guided by standardized protocols jointly established by PNNL, LLNL, and SNL. These carefully curated datasets serve as a crucial foundation for benchmarking and advancing neural operator architectures, while improving their generalization capabilities across diverse scientific applications. PNNL has made significant strides in integrating transformer architectures with neural operators, demonstrating strong capabilities for handling complex geometries. This progress is further enhanced by SNL's expertise in design optimization, incorporating real-world constraints to improve predictive reliability and optimization outcomes. SNL has made progress in performing a comprehensive benchmark of neural operator uncertainty quantification methods under multi-fidelity conditions which will aid in later stages of the project. LLNL has developed novel window functions for hard enforcement of boundary and interface conditions, ensuring robust handling of the constraints. This method will be used to treat heterogeneous systems with interfacial discontinuities such as developing surrogate models for SNL and PNNL's battery data sets.

WHAT THE TEAM IS SAYING

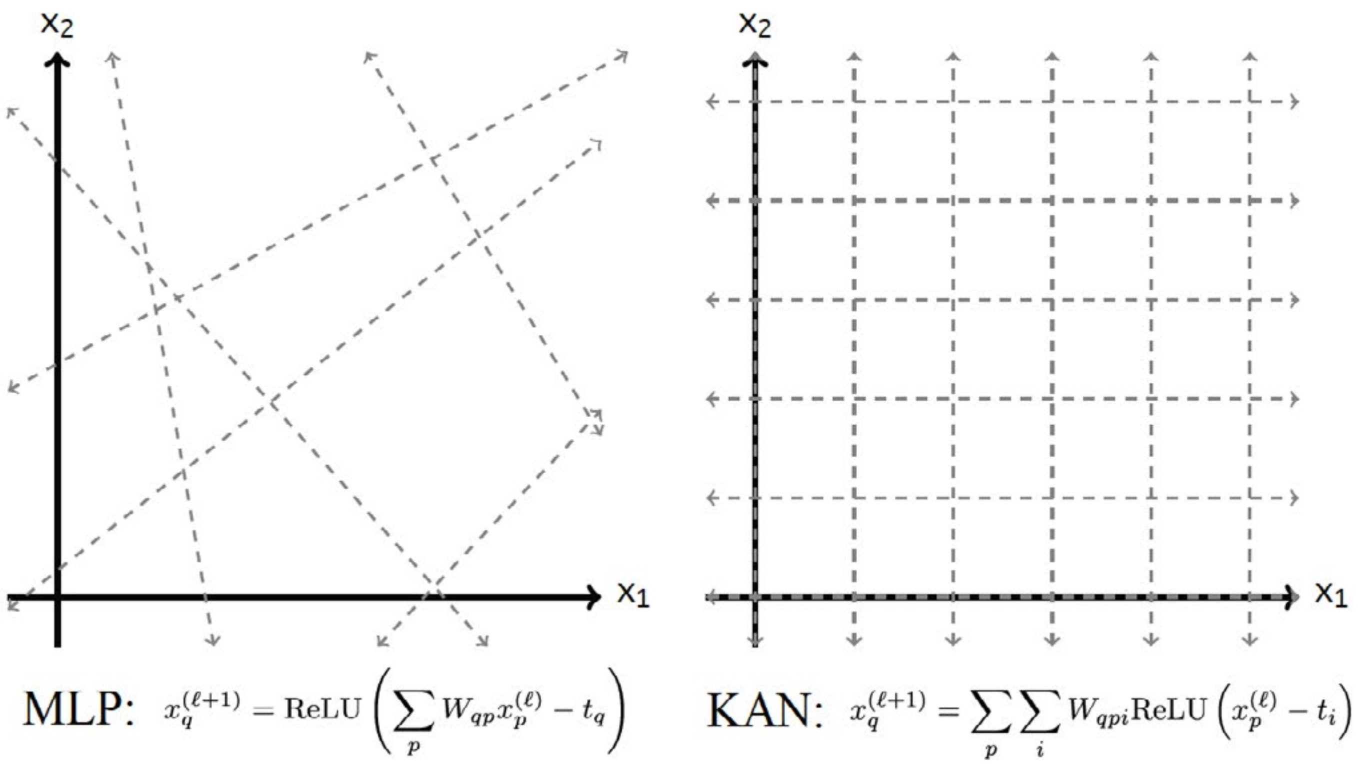
"The IL-LDRD is a unique opportunity for NNSA labs to collaborate beyond our traditional partnerships with non-NNSA labs such as PNNL. PNNL has world class expertise in Scientific Machine Learning (SciML), and it's been great to begin building a larger SciML community in the national lab ecosystem as a whole." – **Michael Penwarden, Sandia**

"This IL-LDRD project is a rare and exciting opportunity to collaborate with experts across LLNL and SNL on advancing AI/ML methods for scientific computing and realworld applications. The structured collaboration fosters innovation and enables impactful outcomes that would not be achievable by any single lab alone." – **Yucheng Fu, PNNL**

"The IL-LDRD offers an excellent platform for collaboration among various laboratories in the field of Scientific Machine Learning. It brings together experts with interdisciplinary backgrounds from SNL, PNNL and LLNL, including core machine learning, uncertainty quantification, computational physics, and experimental science. As a result, the project is indeed an amazing opportunity to exchange ideas and applying those to problems of national importance while advancing the frontiers of physics- and data-driven machine learning." – **Pratanu Roy, LLNL**

MULTILEVEL MACHINE LEARNING FOR PERFORMANCE AND RELIABILITY

LANL PI: BEN SOUTHWORTH
LLNL PI: RUI PENG LI
SANDIA PI: ERIC C. CYR



The image shows cut planes of a classical MLP layer (left) yielding an unstructured approximation, while KANs (right) are semi-structured without suffering from the curse of dimensionality.

This project aims to develop multilevel neural network architectures and training methodologies applied to scientific machine learning applications. We hypothesize that multilevel structure in neural network training and the incorporation of multifidelity data can revolutionize the applicability and reliability of scientific machine learning in scientific mission spaces through dramatic acceleration of training and increased control of model fidelity.

This project started in January of 2025. Since the start of the project, Sandia and Los Alamos have related the Kologomorov Arnold Networks (KANs) to multi-channel multilayer perceptrons (MLPs). The researchers showed that there is a one-to-one mapping between KANs and MLPs. Additionally, by exploiting this relationship the researchers developed a preconditioned gradient descent algorithm that leads to training algorithms for MLPs that yield the feature resolution of KANs. Critically this preconditioner allows for MLPs to overcome spectral bias. Further work showed that by exploiting natural geometry in KANS, a hierarchical training algorithm naturally arises and is an effective approach for reducing computational costs. Los Alamos has also worked on a general framework for linear and nonlinear preconditioned optimization for machine learning in the context of classical methods for numerical partial differential equations. This perspective has facilitated the development of new optimization methods which outperform state-of-the-art methods on simple nonconvex optimization problems and are currently being tested on more complex and high dimensional problems.

LLNL has investigated the spectral bias in neural network-based PDE solvers, specifically Physics-Informed Neural Networks (PINNs) and the Deep Ritz Method (DRM). The LLNL researchers analyze how the loss functions in PINNs and DRM correspond to different Sobolev norms of the solution errors. Through Fourier analysis and visualization of the approximation errors in the frequency domain, distinct spectral biases exhibited by each method are explored. To address these biases, the project team is developing a multilevel, multiscale framework that integrates PINNs and DRM with enhanced Fourier and Chebyshev features. This hybrid approach aims to mitigate the limitations of each method with respect to high-frequency components. Preliminary results on Poisson equations demonstrate the potential effectiveness of our proposed method.

WHAT THE TEAM IS SAYING

“The IL LDRD program provides a real boost to research innovation by combining the considerable strengths of different labs. In our project, this has allowed a rapid transfer of information that has accelerated the development of key mathematical insights.” – **Eric Cyr, Sandia**

“The Interlaboratory program has enabled a formal collaboration with LLNL and Sandia building on many years of informal and unfunded interactions between our team members.”– **Ben Southworth, LANL**

“The Interlaboratory LDRD program provides a valuable opportunity to investigate the fundamental mathematics underlying neural networks as function approximators and PDE solvers. It enables us to bring together a team with diverse and complementary expertise, within LLNL and in collaboration with SNL and LANL, to effectively pursue this interdisciplinary research.”– **Rui Li, LLNL**

Scientific Leadership and Service

Tomi Akindele, Holly Carlton and Kelli Humbird were awarded the Presidential Early Career Award for Scientists and Engineers by President Biden. (Photos: Blaise Douros/LLNL)

Livermore's LDRD principal investigators and research teams have received numerous prestigious honors, awards, and recognition for LDRD-funded work.

THREE LLNL SCIENTISTS HONORED WITH PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

President Biden awarded the Presidential Early Career Award for Scientists and Engineers (PECASE) to nearly 400 distinguished scientists and engineers, recognizing their exceptional contributions and potential for leadership in their research fields in January, 2025. Among the honorees are three distinguished researchers from Lawrence Livermore National Laboratory: Tomi Akindele, Holly Carlton and Kelli Humbird.

Established in 1996 by President Clinton, the PECASE is the highest honor bestowed by the U.S. government on early-career scientists and engineers. The award acknowledges far-reaching developments in science and technology, enhances connections between research and impacts on society, promotes awareness of science and engineering careers, and highlights the critical role of science and technology in shaping the nation's future.

PECASE awardees, including the three LLNL scientists, are at the forefront of scientific innovation and leadership, making substantial contributions to the nation's progress in various scientific fields, according to the White House announcement. Their work exemplifies the impact of dedicated research and collaboration in addressing complex challenges and advancing knowledge.

TOMI AKINDELE

Nuclear engineer Tomi Akindele has been recognized for her pioneering research at the intersection of nonproliferation and particle physics. Her work focuses on advancing the understanding of neutrinos as a tool for reactor monitoring through international scientific collaboration. Akindele's contributions include developing a new scintillator formulation to enhance the detection of neutrino interactions.

"Receiving the PECASE reinforces why I'm so fortunate to have a career at LLNL," Akindele said. "LLNL has been a leader in applied antineutrino detection for decades. The opportunities that led to this award would not have been possible at another institution."

"The dedicated focus on mentorship here has been imperative to my success," emphasizing the importance of collaboration at LLNL. "Although the award is issued to individuals, the work that led to the award could not have been possible without the support of the multi-disciplinary teams I collaborate with."

Akindele received her Ph.D. in nuclear engineering from University of California, Berkeley, and a bachelor's degree in nuclear engineering Texas A&M University. She started at LLNL as a summer student in 2014.

HOLLY CARLTON

Materials scientist Holly Carlton is a group leader in the Materials Engineering Division. Her research explores the process, structure, properties and performance relationship of advanced manufactured materials using advanced characterization techniques. Carlton's work using in-situ mechanical testing of additively manufactured alloys at the Advanced Light Source synchrotron facility led to greater understanding of failure modes and defect tolerances in 3D-printed metal alloys and light-weighted structures. Her work continues to focus on developing a fundamental understanding of mechanical behavior of alloys in challenging areas important to Laboratory programs.

"This award is such an honor. I am incredibly grateful to the mentors, colleagues, and of course my family who have supported me throughout this journey," Carlton said. "I am excited to continue exploring new research directions and contributing to impactful scientific advancements. I look forward to using the grant money to conduct future studies that focus on using advanced manufacturing techniques to create novel materials for fusion energy science applications."

Carlton received her Ph.D. and master's degree in materials science and engineering and a bachelor's degree in engineering physics from the University of California, Berkeley. She joined LLNL as a postdoctoral research scientist in 2012.

KELLI HUMBIRD

Design physicist Kelli Humbird has been recognized for her innovative application of machine learning in inertial confinement fusion (ICF) physics. Her early work involved building a machine learning model on a vast database of 2D ICF simulations, leading to the discovery of a new class of igniting implosions. Humbird's research continues to push the boundaries of machine learning and physics, with applications in nuclear forensics, weapons physics and ML-based accelerators for simulations.

"Receiving the PECASE is a great reminder to reflect on the career I've had so far, so I can be intentional about shaping where I go next," Humbird said.

Emphasizing the importance of passion and teamwork, Humbird offers advice to aspiring scientists. "Do what excites you, even if it's not what others are doing or what they value at the time and surround yourself by people who say 'yes' to new ideas," she said.

Humbird earned her Ph.D., master's and bachelor's degrees in nuclear engineering and a bachelor's in physics from Texas A&M University. She joined LLNL as a summer intern in 2016.

MIT Technology Review has named Lawrence Livermore National Laboratory (LLNL) research scientist Xiaoxing Xia as one of its 2025 Innovators Under 35 — a global list honoring early-career researchers and entrepreneurs who are shaping the future of science and technology. (Graphic: Dan Herchek/LLNL)

LLNL'S XIAOXING XIA NAMED AMONG *MIT TECHNOLOGY REVIEW*'S TOP INNOVATORS UNDER 35

MIT Technology Review has named LLNL research scientist Xiaoxing Xia as one of its 2025 Innovators Under 35 — a global list honoring early-career researchers and entrepreneurs who are shaping the future of science and technology.

The publication recognized Xia in the Inventors category for his groundbreaking advances in developing and deploying two-photon polymerization (2PP) 3D printing — a key fabrication method for building complex microscale structures. His work combines laser pulse shaping with a custom-engineered metalens array, enabling printing that is faster, finer and more versatile than current commercial systems.

Since joining the Laboratory in 2019, Xia has played a key role in multiple Laboratory Directed Research and Development projects, including efforts that bridge additive manufacturing (AM) with high-energy-density physics and inertial confinement fusion (ICF) target production. He leads projects aimed at developing next-generation 2PP technologies that improve throughput, resolution and multi-materials printing capability using a suite of laser-based AM tools to build functional microstructures for applications in quantum computing, microfluidics, energy, responsive materials and ICF.

"I'm honored to be part of this year's Innovators Under 35 cohort," Xia said. "I'm grateful to the collaborators, mentors and entire support team at LLNL who have made our work possible. I really couldn't think of a better place to work at. I am immensely grateful for LLNL's unparalleled research environment for pushing the boundaries of AM and allowing me to explore ideas that would be difficult to pursue anywhere else."

Xia earned his doctoral degree in materials science from the California Institute of Technology. He holds a bachelor's degree in physics and in economics from the University of Chicago. His work spans both experimental and computational domains, drawing on expertise in ultrafast lasers, nonlinear optics and multiphoton polymerization to address technical challenges with national security relevance.

Each year, MIT Technology Review's list highlights 35 innovators under the age of 35 whose work promises to have a profound impact on the world. Xia joins a distinguished group of past recipients, including Nobel laureates and founders of leading technology companies.

LLNL physicist Hye-Sook Park, who has been awarded the Edward Teller Award for 2025, poses in front of the National Ignition Facility. (Image: Jason Laurea/LLNL.)

LLNL PHYSICIST RECEIVES EDWARD TELLER AWARD

LLNL physicist Hye-Sook Park has been awarded the Edward Teller Award for 2025 by the American Nuclear Society. The award recognizes her pioneering high energy density experimental work at NIF in high-pressure materials science, inertial confinement fusion and astrophysical collisionless shock generation, including the resulting particle acceleration and magnetic field generation.

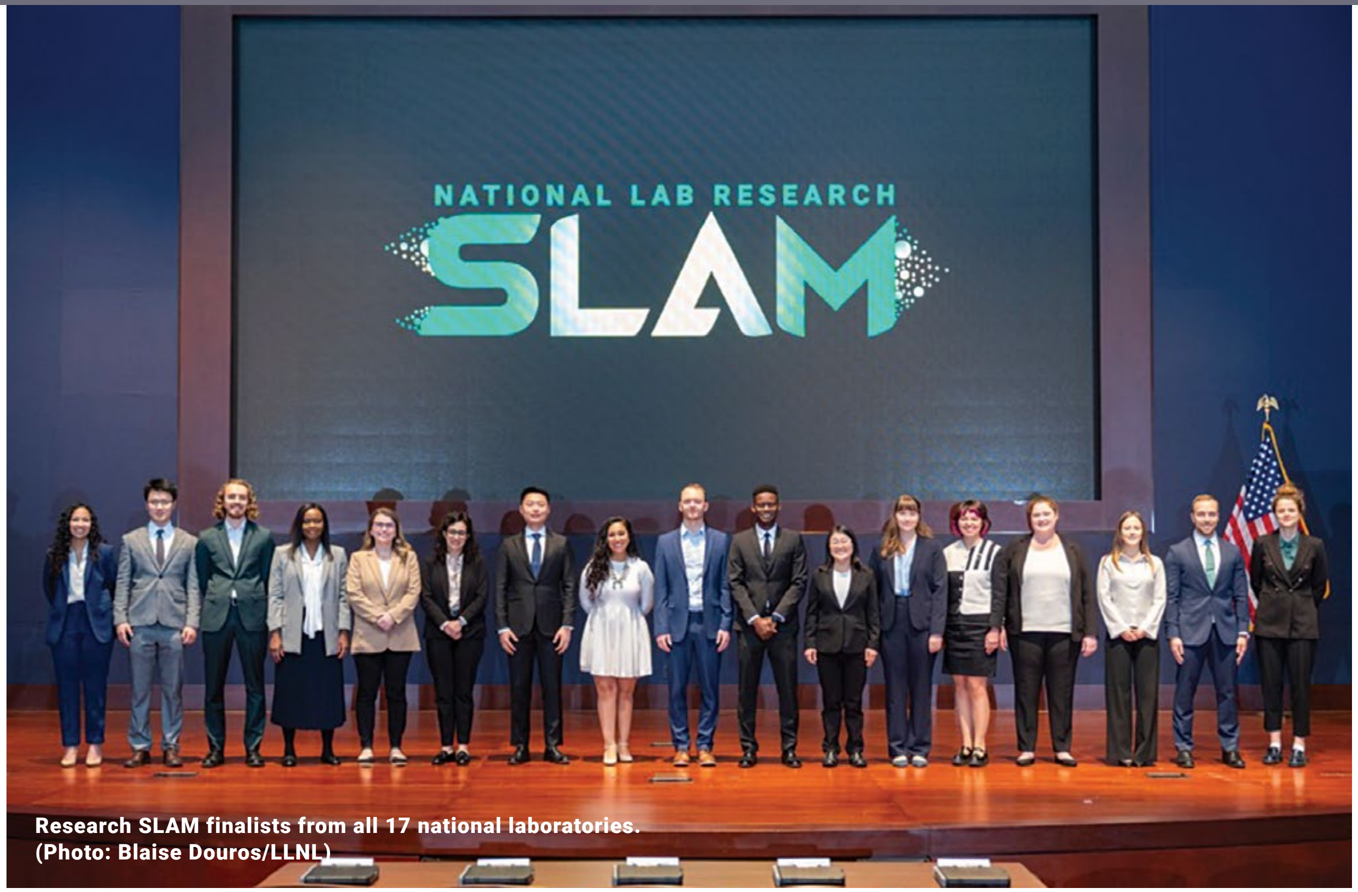
"It is a tremendous honor to receive this award, and I am truly humbled by the recognition," Park said. "The journey to develop new high energy density experimental platforms has been both challenging and deeply rewarding. The process required countless hours of dedication, perseverance and, admittedly, many sleepless nights. Seeing these platforms reach maturity and now consistently produce outstanding scientific results is incredibly gratifying."

The high energy density experimental platforms are being used at NIF to study inertial confinement fusion to reduce undesired target capsule instabilities, material science to understand material properties in extreme high-pressure regimes, and laboratory astrophysics to resolve particle acceleration mechanisms in collisionless shocks.

"This achievement represents not only my personal commitment and enthusiasm over the past two decades, but also the collective efforts of an extraordinary group of individuals," Park said. "I greatly appreciate my mentors, whose guidance has been invaluable; my coworkers, whose collaboration and support have been essential; the high energy density science community, whose shared passion drives innovation; and the entire NIF operational team, whose expertise and dedication have made this research possible."

Since joining LLNL in 1987, Park, a Distinguished Member of Technical Staff, has contributed flight experiments for the Strategic Defense Initiative, led gamma ray burst counterpart search experiments and pioneered radiography techniques using short-pulse lasers to probe thick, high-Z materials. Her research has validated material strength models under extreme conditions. Park is a Fellow of the American Physical Society and recipient of the Dawson Award (2020) and Landau-Spitz Award (2024).

The Edward Teller Award is awarded biennially and recognizes pioneering research and leadership in the use of high-intensity drivers (such as lasers, ion-particle beams or pulsed power) to produce unique high-density matter for scientific research and to conduct investigations of inertial fusion.



Research SLAM finalists from all 17 national laboratories. (Photo: Blaise Douros/LLNL)

NATIONAL LAB RESEARCH SLAM CELEBRATES EXCELLENCE IN SCIENCE, INNOVATION AND COMMUNICATION

Three minutes. One slide. That's all that 17 early-career researchers — each representing one of the Department of Energy (DOE) National Laboratories — had to present their science at the second National Lab Research SLAM on March 5, 2025.

Sponsored by the House Science & National Labs Caucus and the Senate National Labs Caucus, the event took place in the Congressional Auditorium on Capitol Hill in front of an audience of 200 policymakers, congressional staffers and laboratory representatives. The competition, which was livestreamed to over 3,500 additional viewers, aims to highlight the key role and impact of DOE laboratories on the nation's innovation ecosystem.

Finalists vied for awards in five categories: National Security, Energy Security, Scientific Discovery, Environment and People's Choice. Nicholas Cross represented Lawrence Livermore National Laboratory with his presentation, "Predicting critical failure in next-generation batteries."

Olivia Pimentel from Los Alamos National Laboratory captured the award for national security with her presentation, "Packaging the Black Death: macro problem, nano solution." Pimentel also won the People's Choice award, which was voted on by the in-person and virtual audience.

"I think that communicating science so that anyone can understand it allows for inspiration of anybody. It allows for people, especially in the case of national lab research, to understand where their money is going and to see that it's going to really huge, impactful, positive things," Pimentel said. "I am just so floored and inspired by these other scientists. It was a tough competition, and I'm really honored to be with these guys."

In the Energy Security category, Yufan Xu of Princeton Plasma Physics Laboratory received the award for his talk, "Can Terminator 2 help humanity unlock unlimited fusion power?"

"I think everybody's a winner, to be honest. You know, we all present different aspects of the research that we do, and we deliver it on the stage," Xu said. "We try to represent something unimaginable in three minutes. I learned a lot from everybody. So, it's a celebration of the research that everyone does."

Karolina Wresilo from Fermi National Accelerator Laboratory was recognized for her presentation in the scientific discovery category, "Seeing the invisible: can neutrinos explain the origins of the universe?"

"To me, it's a huge accomplishment. Being given the opportunity to present on a national stage, and then also be honored with a win, is extremely important to me," Wresilo said. "Especially as someone who's quite passionate about outreach, I just feel very honored."

In the environment category, Michael Leveille of Sandia National Laboratories was awarded for his talk, "Blend green and flow clean: hydrogen in gas pipelines."

"[Winning this award] means so much. I'm really honored to be able to represent Sandia and to share my research with so many people," Leveille said. "Communication is key — we need to be able to talk about our research and make an impression on someone for it to really have impact. To have the opportunity to take such a big stage, relay a message, and potentially make an impression on so many people — I'm still shocked."

The winners were evaluated based on their comprehension, content, engagement and communication. Results (excepting the People's Choice award) were decided by a panel of esteemed judges:

- **Harriet Kung**, acting director of the Office of Science in the DOE.
- **Theresa Maldonado**, vice president of research & innovation in the University of California Office of the President and president of the American Association for the Advancement of Science.
- **Alton D. Romig, Jr.**, executive officer of the National Academy of Engineering
- **Wendin Smith**, deputy undersecretary for counterterrorism and counterproliferation in DOE.
- **Steve Walker**, vice president & chief technology officer at Lockheed Martin and former director of the Defense Advanced Research Projects Agency.

ON THE COVER

A very detailed "molecular level" picture of the apoferritin protein, taken with a high powered cryo-electron microscope, with enough detail to almost see the atoms.