Annual Report **Overview**

Laboratory Directed
Research and Development
Lawrence Livermore National Laboratory

FY2018

ldrd.llnl.gov

About the Cover

Top image from Adobe Stock. Bottom image: LDRD's early support of research in additive manufacturing has spawned numerous interdisciplinary efforts in Laboratory programs. For instance, researchers have combined high-performance computing and additive manufacturing to design and build new devices and materials with unique physical and microstructural properties, including this design graphic for an octet truss structure created in a novel material using microstereolithography.

Acknowledgments

We at the Laboratory Directed Research and Development Program extend our sincere appreciation to the principal investigators of the fiscal year 2018 portfolio for providing the project summaries for this annual report.

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Annual Report **Overview**

Laboratory Directed Research and Development

Lawrence Livermore National Laboratory

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In a project that made headlines (17-ERD-085), a team of Livermore researchers and collaborators provided experimental evidence for superionic conduction in water ice at planetary interior conditions. When water is heated to several thousand degrees at high pressure, similar to the conditions inside giant planets like Uranus and Neptune, its state is characterized by liquid-like hydrogen ions moving within a solid lattice of oxygen. In other words, it is simultaneously solid and liquid.

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Director's Statement

Lawrence Livermore National Laboratory's (LLNL's) enduring mission to enhance national—and world—security relies on constant innovation in science, technology, and engineering. For nearly thirty years, LLNL's ability to stay ahead of evolving threats has been owed in large measure to the Laboratory Directed Research and Development (LDRD) Program. LDRD helps sustain the Laboratory's role as an incubator for new ideas and formidable engine of scientific discovery.

Congress established the LDRD Program in 1991 to maintain the technical vitality of the Department of Energy national laboratories. Since then, LDRD has continued to be an essential tool for addressing challenges that lie beyond the planning horizon of our programs. Under LDRD, the Laboratory invests a small portion of its total operating budget in areas beyond the scope of traditional programmatic research, where high-risk exploration can lead to big payoffs.

Competition is keen among scientists and engineers for LDRD funding. Projects are selected through a rigorous peer-review process that prizes innovation and creativity, potential impact on a technical field, qualifications of the researchers, and the proposed research approach.

The broad range of projects described in this annual report illustrates the enormous breadth of cutting-edge research LDRD supports, from advanced manufacturing to high-performance computing to a prototype "brain-on-a-chip." The current scientific and technical strengths of the Laboratory are, in large part, a product of past LDRD investments. Many highly successful Livermore programs trace their beginnings to an LDRD-sponsored research effort.

Projects sponsored by LDRD contribute significantly to Lawrence Livermore's intellectual property, publications, and collaborations. In addition, many technologies that come out of the LDRD Program have commercial value; the Laboratory's Industrial Partnerships Office licenses these technologies to the private sector to strengthen U.S. industry.

Because LDRD projects are typically at the forefront of science, they help to attract promising young scientists and engineers working at the state of the art. As an example, LDRD historically supports more than half of Livermore's postdoctoral researchers. The program has also helped other Laboratory scientists establish careers in exciting new research directions.

LDRD-funded efforts have produced enormous payoffs over the past 27 years, and I am confident they will continue to ensure that LLNL's robust science, technology, and engineering base remains a national asset.

William H. Goldstein, Director

How to Read This Report

The LDRD FY18 annual report contains two parts:

1. **The overview.** This section introduces readers to Lawrence Livermore National Laboratory and the LDRD program, describes the program's structure and management, and provides an update on portfolio statistics, scientific accomplishments, and metrics of performance.
2. **Individual project reports.** This section contains detailed final reports of all projects that concluded in FY18. Final reports contain a description of the project's background and objectives; an inventory of the scientific results achieved; and a summary of the impact of the project to DOE, NNSA, and Laboratory missions. References and a cumulative list of the publications and presentations produced over the project's duration are also provided. This section also contains brief descriptions of projects that are ongoing.

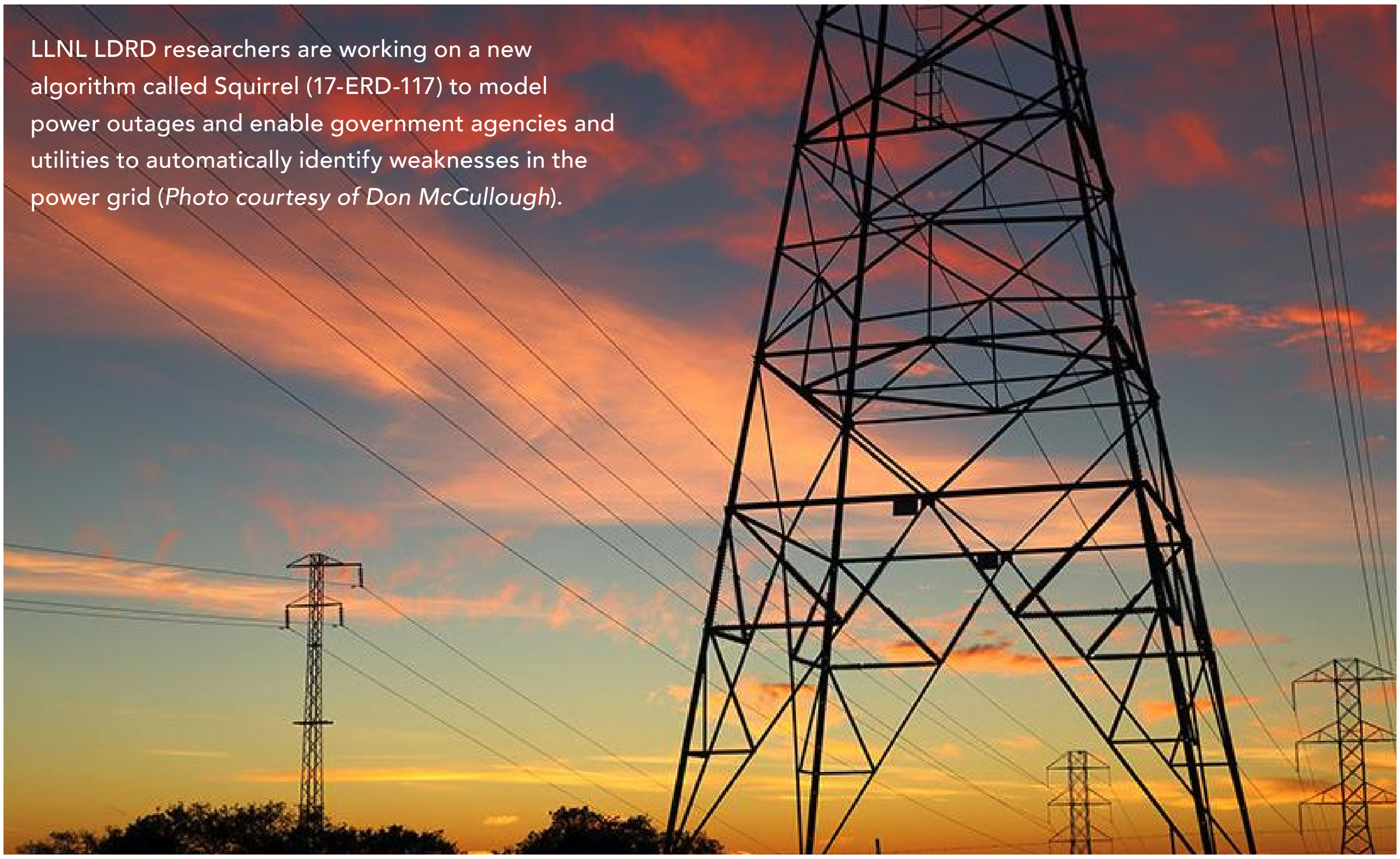
Project reports are organized by field of research and project type, such as feasibility studies, exploratory research, and so on. (See section "Types of Projects" for a complete list of project types and descriptions).

Every project is assigned a three-element tracking code:

- The first element is the fiscal year in which the project began.
- The second represents project type.
- The third identifies the serial number of the project within its fiscal year.

For example, the tracking code "18-FS-001" identifies a feasibility study that began in FY18, with a serial number of 001.

Note that some project reports are withheld from publication due to classification but are available through the appropriate channels.



LLNL LDRD researchers are working on a new algorithm called Squirrel (17-ERD-117) to model power outages and enable government agencies and utilities to automatically identify weaknesses in the power grid (*Photo courtesy of Don McCullough*).

The Laboratory Directed Research and Development Program at LLNL

Congress established the LDRD program at the DOE national laboratories in 1991 to foster excellence in science and technology and to ensure the laboratories are technically vital and prepared to meet today's needs and tomorrow's challenges. LDRD achieves this by supporting high-risk, potentially high-payoff research and development projects. At LLNL, this program provides the most significant resource for internally directed scientific and technical investments.

Program Mission

According to DOE Order 413.2C, the LDRD program serves to

- support the missions, strategic vision, and core competencies of the DOE/NNSA and LLNL;
- maintain the Laboratory's science, technology, and engineering vitality;
- attract and retain the most qualified scientists and engineers and allow scientific and technical staff to enhance their skills and expertise;
- pursue collaborations with academia, industry, and other government laboratories;
- generate intellectual property; and
- strengthen the U.S. economy.[1]

Toward these ends, LDRD funds leading-edge research and development while helping to recruit, train, and mentor top talent in new and emerging fields, typically including, for example, 50% of the Laboratory's postdoctoral researchers, many of whom become career employees who are internationally respected in their fields (see "Awards and Recognition"). LDRD both supports the basic research that is instrumental in enhancing the core competencies of the Laboratory and applies those competencies in novel ways to achieve national security mission goals, often forming the foundation of new programs. Furthermore, with its emphasis on creative science and novel methods, LDRD research often leads to inspired collaborations, intellectual property, and technical innovations that are transferred to industry. (For examples, see "Long-Term Impacts of LDRD Investments.") Altogether, Livermore's technical strength and agility, as well as its status as a premier research institution are, in large part, a product of LDRD investment choices.

Program Leadership

LLNL director William Goldstein and deputy director for science and technology Patricia Falcone were responsible for the Livermore LDRD program in 2018. Execution of the program was delegated to LDRD program director, Doug Rotman. The LDRD program at Livermore complies fully with DOE Order 413.2C and relevant DOE orders and guidelines.

Oversight

The LDRD program achieves continual improvement through internal and external reviews of program management, execution, and oversight of each LDRD project.

In accordance with DOE Order 226.1B[2] of the prime contract between NNSA and Lawrence Livermore National Security, LLC, a contractor-assurance system is in place at the Laboratory; the LDRD office uses this system and the tools provided to support improvements in LDRD program performance.

In May 2016, the director of the Office of Science, Cherry A. Murray, asked the Advanced Scientific Computing Advisory Committee (ASCAC) to perform an independent review of the LDRD program, the purpose being to consider the overall impact of LDRD in four representative laboratories (including Livermore, the sole NNSA facility represented).The ASCAC subcommittee engaged in extensive written dialog with representatives of the chosen LDRD programs and also made site visits to the laboratories. Overall, the ASCAC subcommittee's review was very positive concerning both the LDRD program as a whole and Livermore's program specifically. Their sole recommendation to LLNL concerned the improvement of tracking the long-term impacts of projects. The report observes, "Planned efforts by LLNL to enhance on-going processes for collecting metrics associated with LDRD programs should better allow them to monitor the long-term impact of LDRDs and demonstrate their success. LLNL should discuss these efforts with the other DOE Labs...."[3]

Toward that end, representatives from the LLNL LDRD program are participating in a working group with other DOE/NNSA laboratories to share best practices and discuss strategies for tracking the long-term impact of LDRD investments. Specifically, in FY18, a subcommittee of the working group was formed to

- formulate a strategy to define long-term impacts,
- determine the metrics by which the long-term impact of LDRD investments can be measured,
- assess and select the methods by which such metrics can be tracked, and
- begin cataloging the impact of projects.

Alignment with DOE, NNSA, and Laboratory Missions

Aligning LDRD projects with DOE, NNSA, and Laboratory missions begins with a process to set institutional goals at the Laboratory level by identifying (a) mission-related areas for focal research, (b) the core competencies that support this research, (c) the scientific and technological needs within the areas and the competencies involved, and (d) key topics in fundamental research. Published as the *Investment Strategy for Science, Technology, and Engineering*,[4] this living document is overseen by multidisciplinary

William H. Goldstein (top), Patricia Falcone (middle), and Doug Rotman (bottom).

1. U.S. Dept. of Energy, No. O 413.2C, *Laboratory Directed Research and Development* (Oct. 22, 2015) (Order). https://www.directives.doe.gov/directives-documents/400-series/0413.2-BOrder-C

2. U.S. Dept. of Energy, No. O 226.1B, *Implementation of DOE Oversight Policy* (April. 25, 2011) (Order). https://www.directives.doe.gov/directives-documents/200-series/0226.1-BOrder-b

3. U.S. Dept. of Energy Advanced Scientific Computing Advisory Committee (ASCAC) Subcommittee on LDRD Review, *Final Report to the Committee*, 4th May 2017. https://science.energy.gov/~/media/ascr/ascac/pdf/charges/2017/REPORTLDRDAPRIL17.pdf

4. Lawrence Livermore National Laboratory, internal document, *Investment Strategy for Science, Technology, and Engineering*, January 1, 2019. LLNL-MI-743840.

teams under the guidance of the deputy director for science and technology and is revised annually to respond to evolving mission needs. This document sets the strategic context for the annual LDRD calls for proposals. Other context-defining publications include the DOE's *Strategic Plan, 2014–2018*[5] and the NNSA's *Enterprise Strategic Vision, August 2015*.[6]

At the programmatic level, LDRD portfolio management at Livermore is structured to guarantee alignment with DOE, NNSA, and Laboratory missions. The structure involves

- calls for proposals that underscore the requirement that projects align with DOE/NNSA missions,
- guidance to prospective applicants on how to work with the aforementioned publications to address DOE/NNSA mission needs in their proposals, and
- a peer-review process for strategic relevance and technical content to select the highest-quality LDRD portfolio from these proposals.

By adhering to the guidance of key documents and the program's portfolio management structure, the Laboratory's 2018 LDRD program strongly supported DOE/NNSA goals in nuclear and national security and scientific discovery and innovation, as in years past.

Topics of Inquiry

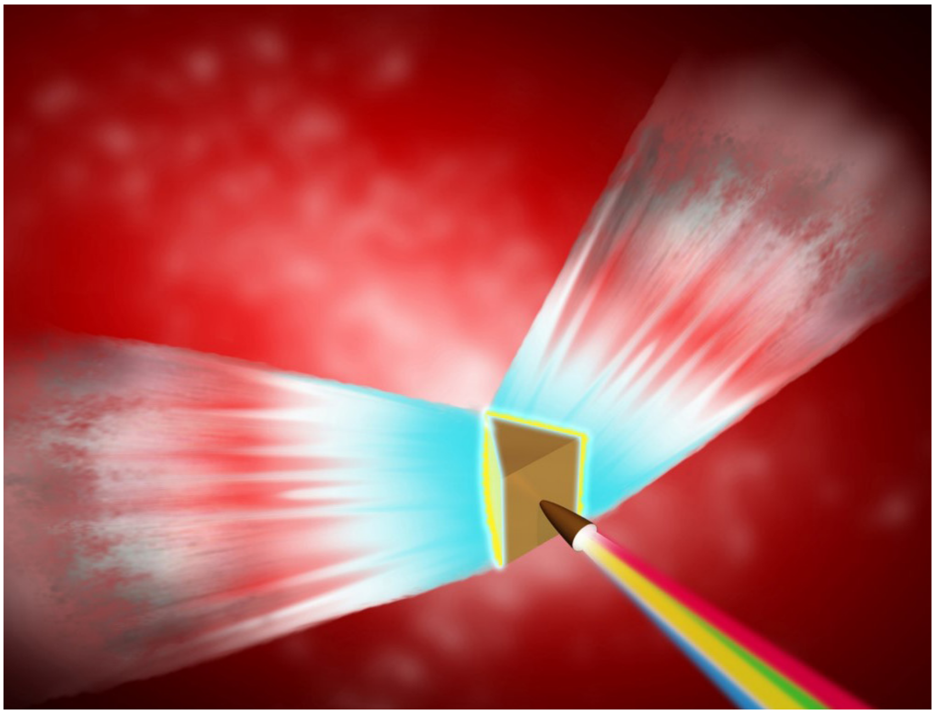
Although LDRD projects frequently invoke more than one scientific discipline, each project is assigned to one of sixteen general categories identified in the Laboratory's science and technology investment strategy. These categories consist of nine mission-driven research and development challenges and seven core competencies (the scientific and technical skills, abilities, and knowledge the Laboratory must command to address the research challenges).

The nine research and development challenges are as follows:

1. **Chemical and biological countermeasures.** Provide innovative systems and capabilities to rapidly detect and effectively respond to intentional use of pathogens and chemical agents, as well as natural outbreaks of pandemic diseases.
2. **Cybersecurity and cyberphysical resistance.** Advance cyber and network science to support U.S. cyber superiority and ensure the resilience of the complex cyberphysical systems throughout the nation's critical infrastructure.
3. **Directed energy.** Develop compact, robust, efficient high-average-power lasers with high optical quality for a broad range of national security applications.
4. **Energy and climate security.** Apply innovative science and cross-cutting energy and climate-change-adaptation technologies to assure national energy and resource security.
5. **Forensic science.** Advance the state of the art in chemical, biological, radiological, nuclear, and explosive sciences to support a broad set of national security needs.
6. **High-explosive physics, chemistry, and material science.** Improve our understanding and prediction of high-explosive behavior to cost-effectively refurbish and enhance the safety of the U.S. nuclear deterrent and counter emerging high-explosive and nuclear threats.
7. **Nuclear threat reduction.** Develop innovative technologies and systems to prevent, detect, counter, and respond to the use or threatened use of nuclear weapons or weapons-scale usable materials.
8. **Nuclear weapons science.** Provide scientific and technological innovation to ensure the safety, security, reliability, and effectiveness of the nation's nuclear weapons stockpile.
9. **Space security.** Develop new capabilities to meet national challenges in space situational awareness, intelligence, surveillance, and reconnaissance.

The seven core competencies are in the following areas:

1. **Advanced materials and manufacturing.** LLNL strives to meet NNSA and broader national needs for the rapid, cost-effective development of advanced materials and manufacturing processes and systems.
2. **Bioscience and bioengineering.** Researchers work at the interface of biology, engineering, and the physical sciences to address national challenges in biosecurity, chemical security, bioenergy, and human health.
3. **Earth and atmospheric science.** Scientists and engineers provide expertise in earth and atmospheric science with high-performance computing to meet national security, energy



LLNL LDRD researchers developed a unique laser-based method for generating the intensity necessary to produce relativistic electron–positron pair plasmas—a form of antimatter that was a major component of the early universe (17-ERD-010). Specifically, they used a special gold cone through which four ARC beams were channeled. This method has application to x-ray diagnostics in stockpile stewardship and nuclear security research.

security, and environmental security needs.

4. High-energy-density science. LLNL provides international leadership in studying and controlling matter under extreme conditions of temperature and pressure.
5. High-performance computing, simulation, and data science. Scientists and engineers support mission needs by advancing high-performance computing to understand and predict the behavior of complex systems, which includes providing leadership in the technically challenging drive toward exascale-class computing; developing and applying higher fidelity and increasingly realistic and reliable science and engineering simulations; and creating scalable capabilities to manage and recognize patterns in big data.
6. Lasers and optical science and technology. This competency entails designing, building, and reliably operating complex laser systems that dramatically advance the state of the art to meet important national needs.
7. Nuclear, chemical, and isotopic science and technology. To support stockpile stewardship and nuclear threat reduction, researchers develop innovative capabilities for nuclear measurements and rare-event detection, and they provide unique resources for chemical and isotopic analysis of samples for wide-ranging research activities.

Types of Projects

LLNL LDRD projects are of four types: strategic initiatives, exploratory research projects, feasibility studies, and Laboratory-wide-competition projects. Each type has its distinctive purpose, duration, and funding limits.

Strategic Initiatives (SI)

The purpose of an SI project is to achieve a leap forward in answering key science, technology, and engineering challenges identified in the Laboratory's investment strategy. The Laboratory director takes an active role in selecting projects, monitoring progress, and disseminating results. An SI project is usually large in scope, typically funded for up to three years at $1.5 to $3M per year, and conducted by a large, multidisciplinary, cross-organizational team of scientists and engineers.

Exploratory Research (ER)

An ER project typically engages a multidisciplinary, cross-organizational

5. U.S. Dept. of Energy, *Strategic Plan*, 2014-2018.
https://www.energy.gov/sites/prod/files/2014/04/f14/2014_dept_energy_strategic_plan.pdf

6. U. S. Dept. of Energy, Natl. Nuclear Sec. Admin. *Enterprise Strategic Vision*, August 2015.
https://www.energy.gov/sites/prod/files/migrated/nnsa/2017/11/f45/Final_Strategic_Vision_2015_9-3_screen%20quality.pdf

team of scientists and engineers in innovative R&D for the purposes of (1) forging a new direction for an existing program, (2) responding to a research challenge within a mission area, or (3) making a breakthrough that enlarges the Laboratory's core competencies and scientific reputation. ER projects, which are the majority of LDRD projects, are funded for up to three years, with an annual budget between $300K and $1.3M per year.

Feasibility Studies (FS)

An FS provides a flexible way for researchers to propose small, short-term projects to determine the feasibility of a particular technical approach to a mission-relevant science and technology challenge. Feasibility studies are limited to a year in duration, with a maximum funding of $175K.

Laboratory-Wide (LW) Competition

LW projects emphasize innovative basic research and out-of-the-box thinking. To encourage the innovation and creativity of individual researchers, the LDRD program requires neither filtering by management nor alignment with the Laboratory's investment strategy, though alignment with DOE missions is mandatory. LWs are typically funded up to $275K per year for two years.

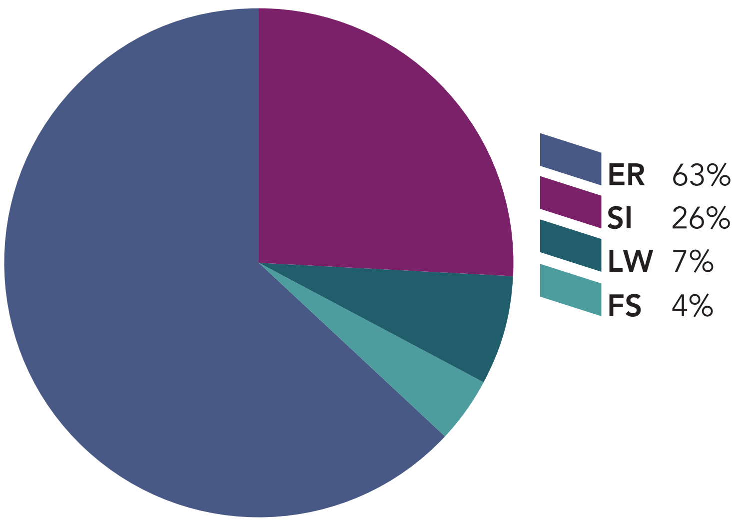
Structure of the FY18 Portfolio

The FY18 portfolio was carefully structured to promote the program's vigorous strategic vision and the long-term goals of DOE, NNSA, and Livermore. The projects in the present annual report underwent stringent peer-review selection and continuous management oversight. In FY18, the LDRD program funded 235 projects, for a total allocation of $98M.

Project Type Distribution

The distribution of funding among the project categories is shown in the following pie chart.

Percentage of Funding by Project Type



Strategic Initiatives. Thirteen SI projects were funded in FY18. Although SIs represented 6% of the total number of LDRD projects for the year, they claimed 26% of the budget. Individual SI projects received funding between $1.6M and $2.6M, with average funding of $1.9M.

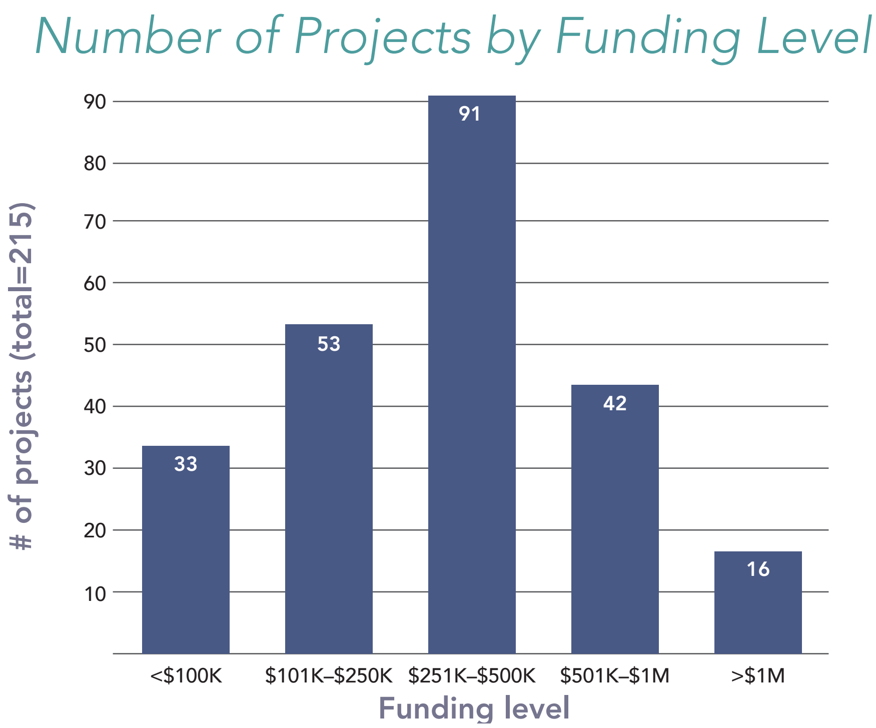
Exploratory Research. In FY18, 155 ER projects constituted 66% of LDRD projects and almost 63% of the budget, making this category the largest in the portfolio. The average allocation for ER projects that were funded for the entire year was about $426K.

Laboratory-Wide Competition. Twenty-six LW projects were funded in 2018, representing 11% of the projects for the year and 7% of the budget. Individual LW projects were allocated an average of about $252K.

Feasibility Studies. The program funded 41 feasibility studies in FY18, accounting for over 17% of all LDRD projects and over 4% of the budget. Many of these studies, which are limited to twelve months in duration, were funded for only part of the year because they began midyear in FY17 (and thus extended into FY18) or midyear in FY18 (in which case they will extend in FY19). Individual studies funded for the full fiscal year received an average of about $100K.

Funding Distribution by Dollar Amounts

The following bar chart shows the distribution of funding by dollar amount, rounded to the nearest $1K increment, for all projects. Of all LDRD projects,14% received less than $100K, while about 22% received $100K–$250K. The largest cluster (39%) was in the $250K–$500K range. Projects in the $500K–$1M range accounted for 18% of the total; 7% received more than $1M. The average funding level was about $418K.



Distribution by Research Topic

The following chart breaks down the number of projects in each field of research and their percentage of LDRD funding. The two largest categories (advanced materials and manufacturing and high-performance computing, simulation, and data science) each garnered about 18% of overall funding, with 33 and 32 projects, respectively.

Projects by Topic

# of projects	Total $K	Topic	
32	18,043	High-performance computing, simulation, and data science	18.3%
33	17,396	Advanced materials and manufacturing	17.7%
31	12,289	Bioscience and bioengineering	12.5%
19	11,548	Lasers and optical science and technology	11.7%
42	11,378	High-energy-density science	11.6%
18	6,201	Nuclear, chemical, and isotopic science and technology	6.3%
13	3,533	Nuclear weapons science	3.6%
3	2,698	High-explosives physics, chemistry and materials science	2.7%
11	2,693	Energy and resource security	2.7%
7	2,439	Space security	2.5%
3	2,284	Forensic science	2.3%
5	2,273	Directed energy	2.3%
7	2,129	Earth and atmospheric science	2.2%
4	1,715	Cyber security and cyber physical resilience	1.7%
1	895	Chemical and biological countermeasures	0.9%
6	815	Nuclear threat reduction	0.8%

0% 5% 10% 15% 20%

Metrics

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

For instance, in FY18, LDRD costs at Livermore were $98.2M, 5.9% of the total Laboratory base; yet LDRD yielded approximately half the Laboratory's patents. This section presents annual performance indicators specified by the Director of the Office of Science for LDRD at the DOE/NNSA laboratories, in accordance with DOE Order 413.2C.

Intellectual Property

Year after year, projects sponsored by LDRD achieve a disproportionate percentage of the patents and copyrights issued for LLNL research. As illustrated in the following tables, LDRD has been key in developing nearly half of the Laboratory's patents, over a quarter of the Laboratory's copyrights (chiefly computer codes), and about half of the Laboratory's records of invention.

Patents	FY14	FY15	FY16	FY17	FY18
All LLNL patents	105	96	97	88	79
LDRD patents	46	46	54	55	41
LDRD patents as a percentage of total	44%	48%	56%	63%	52%

Records of Invention	FY14	FY15	FY16	FY17	FY18
All LLNL records	86	122	91	110	105
LDRD records	45	65	43	53	47
LDRD records as a percentage of total	52%	53%	47%	48%	45%

Copyrights	FY14	FY15	FY16	FY17	FY18
All LLNL copyrights	76	68	72	105	105
LDRD copyrights	23	21	19	19	23
LDRD copyrights as a percentage of total	30%	31%	26%	18%	22%

Scientific Publications

Laboratory scientists and engineers publish over a thousand papers each year in a wide range of peer-reviewed journals, of which LDRD-funded work consistently accounts for a large portion. For each year listed in the following table, the number of LDRD-derived publications should be considered a minimum value and the true value larger, because the long-term impact of

LDRD investments is manifest in publications that may appear long after the project has ended.

Journal Articles	FY14	FY15	FY16	FY17	FY18
All LLNL articles	985	1,010	1,041	1,126	1,178
LDRD articles	245	265	265	274	456
LDRD articles as a percentage of total	25%	26%	25%	24%	39%

Collaborations

External collaborations are essential to the conduct of research and development in LDRD. By working formally and informally with other national laboratories, academia, and industry, LDRD investigators access leading facilities and knowledge in the U.S. and abroad. Recent data on formal collaborations, defined as those in which an external collaborator received LDRD funds from LLNL, are given in the following table. Informal collaborations, in which the LLNL principal investigator and team intend to publish their work jointly with external collaborators, provide an indication perhaps of the broad intellectual engagement and scientific benefit of LDRD collaboration.

Collaborations	FY14	FY15	FY16	FY17	FY18
Projects with one or more formal collaborations	39	31	45	62	74
Percentage of all projects	27%	20%	25%	29%	31%

Students and Postdoctoral Researchers

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 table, LDRD investments contribute to the health and robustness of LLNL's student and postdoctoral researcher programs.

Students and Postdoctoral Researchers	FY14	FY15	FY16	FY17	FY18
Students supported by LDRD	67	102	102	127	138
Percentage of all students	18%	23%	19%	22%	22%
Postdoctoral researchers supported by LDRD ≥10% of thier time	95	102	107	137	167
Percentage of all postdoctoral researchers	68%	43%	39%	44%	54%
LDRD postdocs converted to full staff	27	35	25	31	52
Percentage of all conversions	68%	90%	69%	53%	71%

Research Highlights

This section provides a sampling of research projects from this year's portfolio, representing a range of categories and various stages of completion. For reference, project numbers that begin with 16 were launched in 2016 and are now complete; those beginning with 17 or 18 were launched in 2017 or 2018, respectively, and are most likely continuing.

Project 16-SI-002: Forensic Science of Genetically Variant Peptides

Principal investigator: Bradley Hart

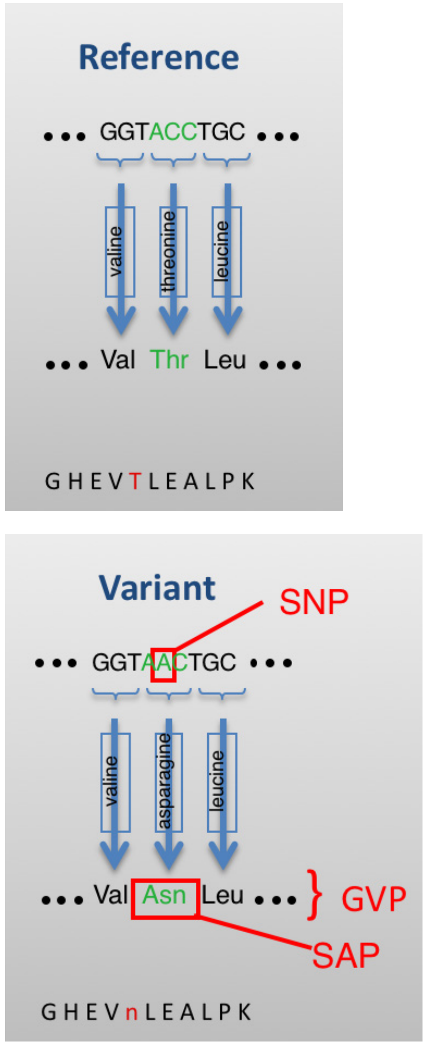
Mission or competency: nuclear threat reduction; forensic science

Executive summary: To address major gaps in forensic science, researchers have developed an entirely new approach to human identification that does not rely on DNA.

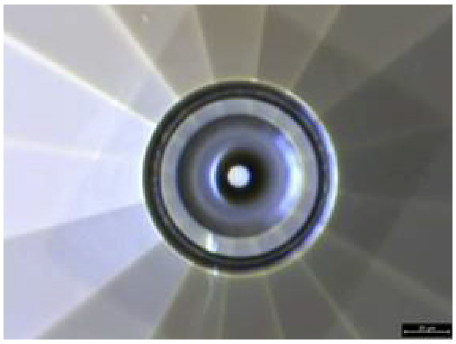
The primary goals of this effort were to develop the foundational science to enable high-fidelity proteomic analysis of hair samples. Human hair contains minimal intact nuclear deoxyribonucleic acid (DNA) for human identification in forensic and archaeological applications. In contrast, proteins offer a pathway to exploit hair evidence for human identification, owing to their persistence, abundance, and derivation from DNA. (i.e., Proteins are chemically more robust than nuclear DNA, and although people do not inherit proteins, they do inherit the DNA that produces their proteins.) Researchers identified variants in proteins resulting from amino acid substitutions that stem from DNA mutation. These variants, known as single amino acid polymorphisms (SAPs), can be used together to generate identifying information about an individual, either in modern forensic or in bioarcheological contexts.

The research conducted in this project has established an entirely new approach to human identification that does not rely on DNA. Furthermore, though the focus was on high-fidelity proteomic analysis of hair samples, the research team has already adapted these methods for use in analyzing bone samples. Often bone is the only remaining human material available to a forensics investigator or bioarcheologist.

Mission Impact: One possible important application for using protein markers from human bones could be to help determine the identity of partial remains from catastrophic events, such as plane crashes, fires, or the 9/11 terrorist attacks. This novel forensic method can also be extended to other security contexts, including counterproliferation, counterterrorism, and homeland security.



Protein primary structure is determined by three base codons in DNA. Mutations within the DNA sequence (a single nucleotide polymorphism or "SNP") can result in alternate amino acids being included in a protein sequence (a single amino acid polymorphism or "SAP"), which provides observable genetically variant peptides (GVP).



Optical microscopy image of the toroidal diamond anvil.

Project #17-ERD-038: Investigation of Ultrahigh-Pressure Phase Transitions in Metals with a Toroidal Diamond Anvil Cell

Principal investigator: Zsolt Jenei

Mission or competency: high-energy-density science

Executive summary: Using newly designed diamond anvil cells, researchers are providing high-accuracy equation-of-state data for metals under extreme pressures and developing new experiment-based understandings of the physics driving material transitions.

The diamond anvil cell, which has been around for over 50 years, has been the primary tool for routinely studying materials up to pressures of about 3 million atmospheres. Static pressures exceeding 4 million atmospheres are extremely challenging to achieve—and experiments reporting these pressures are rare—but they are necessary for the study of matter that exists under these conditions in natural environments, such as planetary interiors. As described in a recent paper published in *Nature Communications*, a team of researchers has demonstrated that a diamond anvil with a toroidal profile is capable of sustaining pressures of over 6 million atmospheres. In their design, the toroidal profile prevents gasket overflow and provides a means to stabilize the central cutlet, allowing a maximum pressure previously accessed only by double-stage diamond anvils and dynamic compression platforms. This optimization of single-crystal diamond anvil design is key in extending the pressure range over which studies can be performed in the diamond anvil cell.

Mission Impact: This research supports nuclear stockpile stewardship science and high-energy-density science by expanding capabilities at the leading edge of static high-pressure science and providing validated tools for measurement of materials of interest. This technology has applications to DOE missions in science, energy, and nuclear security.

Livermore chemist Anna Belle holds a sample case of chemical biosensors she fabricated for measuring neurotransmissions in the brain. (Photo by Randy Wong/LLNL)

Project # 16-ERD-035: The Engineered Micro-Sensor Array

Principal investigator: Anna Belle

Mission or competency: bioscience and bioengineering

Executive summary: Researchers have developed a first-of-its kind chemical sensor platform that will allow for the long-term study of the body's response to bio-agents and drugs.

Biological systems communicate and function through a series of complex biochemical and electrical interactions. The ability to monitor these diverse interactions in real time and in physiologically relevant settings can be a powerful tool in determining the biological causes of diseases and uncovering the mechanisms underlying the body's response to chemical agents. While there are abundant electrical recording instruments, there are few chemical recording platforms. This is despite the fact that only a fraction of the body's signaling mechanism is electrical and the majority is biochemical. Over 500 quadrillion chemical reactions occur in our bodies each day. The goal of this project was to provide a fundamental understanding of the body's response to bio-agents and drugs by developing an advanced chemical-sensor platform. A team of scientists and engineers have developed individual sensors to monitor cell health by measuring multiple biomarkers simultaneously, in real time. They first created a sensor array and the recording instruments needed to build this advanced sensor platform. Then they addressed the problems of sensor lifetime by using a novel technique of chemically engineering enzymes with nanometer-scale complexes that improve enzyme stability. To improve sensor sensitivity, they custom engineered strings of nucleotides to specifically recognize complementary strings of nucleotides on target proteins of interest and also increased the electrode sensing interface with a custom roughening technique. Finally, they enhanced the fabrication of the electrode arrays by incorporating carbon-based materials into the micro-fabricated array platform, thereby opening the possibilities for new sensor methods on the platform. As a result, this platform allows, for the first time, the long-term study of the acetylcholine neurotransmitter system affected by nerve agents and open doors to sense protein-based biomarkers important to monitoring immune response. It also makes nondestructive chemical sensing accessible to the two- and three-dimensional biomolecular platforms that will be commonplace in the near future.

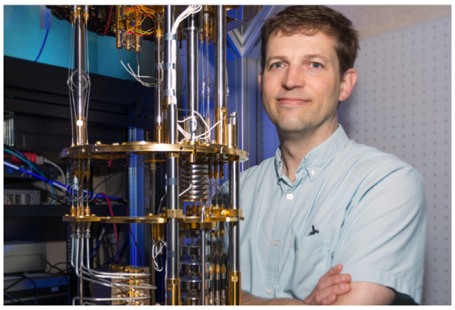
Mission impact: These chemical sensors are a rapid, nondestructive method for monitoring cell health that enables the development of countermeasures against biological and chemical threats. These sensors can also be modified to enable electrochemical detection both in a clinic and in the field.

Project #16-SI-004: Enhanced Coherence for Quantum Sensing and Simulation

Principal investigator: Jonathan DuBois

Mission or competency: advanced materials and manufacturing; cybersecurity and cyber-physical resilience

Executive summary: To address challenges in cyber-physical resilience, researchers have developed a robust capability to design, fabricate, and characterize quantum coherent devices for applications in sensing and analog quantum simulation.



Among the numerous achievements of this project was the development of a full-stack quantum testbed platform capable of probing and controlling quantum systems at a few thousandths of a degree above absolute zero temperature.

Researchers have developed a robust capability to design, fabricate, characterize, and optimize the performance of quantum coherent materials and devices for applications in sensing, analog quantum simulation, and quantum computing. The team has also made significant contributions to the understanding and amelioration of noise sources in superconducting quantum circuits, developed and implemented the skill sets required to design and fabricate novel quantum sensors and quantum computing devices, and formed strong partnerships with leading groups in academia, industry and other national laboratories to further the development and application of quantum devices and materials. The key technical accomplishments resulting from this project include the following:

- establishment of world-class quantum materials and quantum computing testbed laboratories
- development and testing of novel quantum computing architectures optimized for near-term applications in scientific quantum computation and simulation
- demonstration of novel applications of advanced manufacturing methods for quantum sensing and materials
- development of new quantum sensing platforms designed to probe the materials sources of quantum decoherence in quantum devices
- demonstration of a multiplexed readout of cryogenic detectors for high-resolution spectroscopy
- discovery of new quantum materials properties in topological insulators (TI) and emergent superconductivity in composite TI and normal metal structures
- realization and application of a novel control-centric approach to efficient realization of quantum algorithms on current and near-term quantum computing hardware

Mission Impact: This research developed new approaches to applying quantum coherent systems to NNSA mission-relevant computational challenges. Future development of quantum computing and simulation has the potential to dramatically impact the nation's stockpile stewardship program through improved computational fidelity and efficiency. Continued research focused on co-design of quantum hardware and hardware-aware quantum algorithms is now sponsored by the DOE Office of Science Advanced Scientific Computing Research (ASCR) under the "quantum testbed pathfinder" program, as well as the NNSA's Advanced Simulation and Computing (ASC) program under the "Beyond Moore's Law" program.

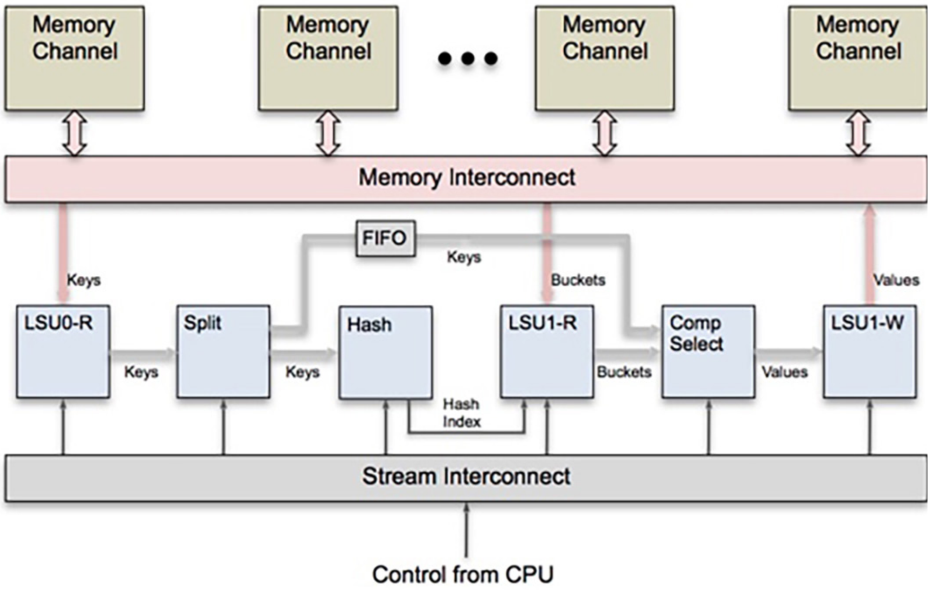
Project 16-ERD-005: In-Memory Associative Indexing: An Approach to Efficient High-Performance Computing

Principal investigator: Maya Gokhale

Mission or competency: high-performance computing, simulation, and data science

Executive summary: Researchers have developed hardware modules that address a long-standing, memory-bottleneck problem in high-performance computing. This novel approach to memory creates efficiencies in performance and energy use, supporting the large computational tasks that underpin many NNSA missions and the design of future exascale architectures.

The memory wall—the growing disparity of speed between a central processing unit (CPU) and the memory capacity outside the unit's chip—is perhaps the most prominent obstacle to processing



A hash table is a data structure that can implement a means for mapping keys to values and placing a data index into an array of buckets or slots, from which a desired value can be found. The lookup accelerator retrieves table entries by streaming hash table indices through a sequence of hardware building blocks including load store units (LSU), a hash unit, and a compare unit that selects the requested keys. Near-memory hardware acceleration delivers up to 12.8 times the performance of equivalent operations in the main processor.

expanding volumes of data. While technological improvements continue to increase the number of processing cores on a chip, improvements in memory bandwidth (i.e., the rate at which data can be read from or stored in a semiconductor's memory by a processor) and memory latency (i.e., the time between initiating a request for a byte in memory until it is retrieved by a processor) at the equivalent scale are not forthcoming, resulting in teraflop-sized supercomputer cores that must sit idle while waiting on data input. If the data are not in the processor's cache, it takes longer to obtain them because the processor will have to communicate with the external memory cells. It is a continuing challenge to keep the CPU cores doing useful work because memory-bandwidth improvements such as high-bandwidth memory mainly benefit regular, streaming access patterns.

A team of researchers addressed the issues of memory latency, bandwidth, and computational power for associative-indexing applications by incorporating key-value store search capabilities into the memory itself. Commonly employed in data science and simulations, particularly in scientific computing that incorporates sparse data structures, this associative-indexing technique is used in search methods wherein data is accessed by content rather than directly accessed by the memory address where the data is stored. The team designed, prototyped, and evaluated a key-value store lookup accelerator optimized for in-memory search. Incorporating logic with memory has become feasible with the emergence of three-dimensional memory stacks that put a memory controller in a base logic layer. In contrast to conventional key-value search accelerators that embed CPUs in the memory, this novel approach created a customized hardware pipeline in the memory itself to search the key-value store. This memory-based accelerator outperformed conventional key-value store search by as much as twelve times. The team evaluated the use of the accelerator in future memory systems using hardware-based emulation.

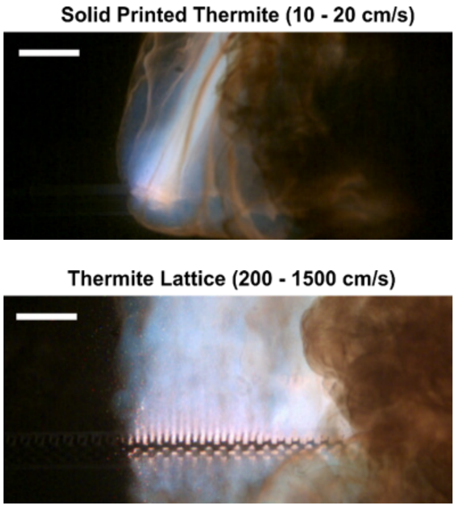
Mission Impact: This research is highly relevant to DOE post-exascale architectures, addressing the memory access bottleneck through research into specialized acceleration functions for scalable compute-node performance improvement. Also, this project resulted in a patent for a near-memory data reorganization engine.

Project 16-ERD-040: Controlling Detonative Phenomena with High-Explosives Material Architecture

Principal investigator: Alex Gash

Mission or competency: high-explosives physics, chemistry, and material science; advanced materials and manufacturing

Executive summary: Researchers developed novel fabrication techniques using dynamic characterization and modeling to capture the unique behavior associated with microscopically designed high-explosive materials. Results enable innovative concepts for surety of stockpile modernization and provide novel energetic material solutions to challenges relevant to conventional defense.



Comparison of printed thermite reaction modes. On top, "fully dense" thermite (printed with no engineered porosity) propagates slowly and exhibits a relatively narrow flame front. On bottom, thermite lattices propagate up to two orders of magnitude faster and show a much broader flame zone led by a front of hot gasses and particles. The scale is the same in both images (scale bar = 1 cm).

Researchers investigated the application of three-dimensional material printing (3DP) to energetic materials (e.g., explosives and pyrotechnics). The initiation and energy release properties of these materials can be highly dependent on the materials' micron-scaled structure and composition. Conventional energetic materials processing provides no engineering control of material architecture on this length scale. Selected 3DP techniques do provide engineering control at the scale of 10s–100s of microns, which enables

a new parameter to the control of performance and safety characteristics. The team developed custom 3D-printable energetic feedstocks and used 3DP techniques to fabricate energetic materials with material architectures that were engineered to have spatially modulated density, structure, and or composition. This approach allowed the systematic investigation of the influence of these characteristics on the initiation and energy release properties of both pyrotechnics and explosives. This development enabled the correlation of select material architectures of a pyrotechnic for energy release rate and linear combustion velocity, as well as substantial control of those properties. For the field of high explosives (HE), this study demonstrated that discreetly placed localized aluminum powder can augment the pressure profile and detonation reaction to lengthen and shift the secondary pressure peak observed in aluminized explosives. Finally, this study showed that topology optimization and engineering of the material composition of the interface between two explosives using 3DP methods is a new and viable tool for engineering the performance of energetics.

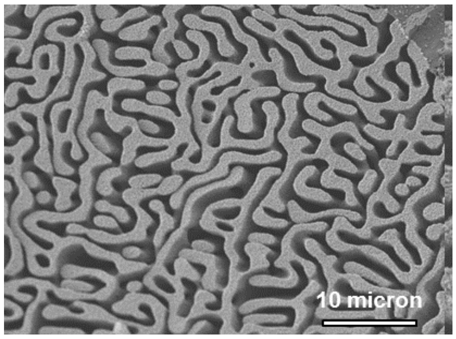
Mission Impact: This project supports national goals in stockpile stewardship and national security while enhancing the Laboratory's advanced manufacturing capabilities. Specifically, the manufacturing methods developed during this project will enable a more detailed understanding of new energetic material architectures, which will support a more innovative design process for components, leading to improvements in the performance, safety, and precision of both the nuclear and conventional stockpiles.

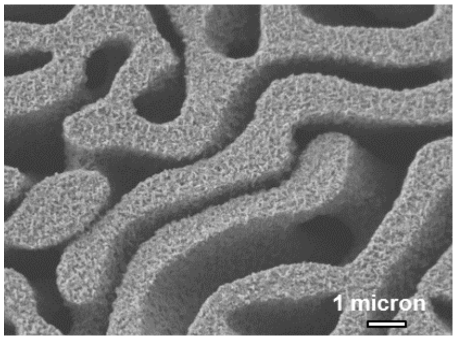
Project 17-LW-013: Hierarchical Nanometer-Scale Porous Copper Flow-Through Electrodes for Efficient Carbon Dioxide Reduction

Principal investigator: Monika Biener

Mission or competency: energy and resource security; advanced materials and manufacturing

Executive summary: researchers developed novel copper membranes with nanometer-scale surface features with which to build electrodes that will function as catalysts in the reduction of carbon dioxide.





Scanning electron micrographs of hierarchical nanoporous copper prepared by dealloying CuAl2 in NaOH.

Researchers explored a flow-through electrochemical reactor design for high-power-density applications. They used pressure-driven mass transport of reactants through bulk porous electrodes to overcome mass-transport limitations and exploit the large internal surface of the designed electrode materials. The electro-catalytic conversion of CO_2 to fuels on porous Cu electrodes was chosen as a test reaction, but the flow-through electrode concept can, in principle, be applied to any other electrochemical transformation for which high power densities are desired. Preferably, the flow-through working electrode has a hierarchical pore morphology: Large pores warrant fast mass transport through the electrode at relatively low pressure differentials across the electrode, and small pores provide the high surface area necessary for achieving high conversion rates for even low reaction probabilities. Unlike flow-by electrolysis setups, the reactant stream is continuously moved *through* the porous catalyst electrode. The team's experiments show that flowing electrolyte solution directly through the electrode increases the CO_2 reduction-related current; however, the effect is small in aqueous electrolytes, owing to the dominance of the competing hydrogen evolution reaction.

Mission Impact: This project advances the DOE goal of delivering tools that support a more economically competitive, secure, and resilient energy infrastructure and addresses LLNL's energy and resource security research and development challenge by providing a pathway to efficient CO_2 capture via oxidative reduction to hydrocarbons using excess energy from regenerative power sources. This research also strengthens the Laboratory's core competency in advanced materials and manufacturing by adding new material synthesis and characterization capabilities. This was the first project at LLNL on electrocatalytic conversion of CO_2 to fuels, which is now a key component of the Laboratory's carbon initiative. It provided the seed for several larger funded projects in this field, including a cooperative research and development project.

Awards and Recognition

LDRD projects are defined by their mission-driven creativity, a characteristic that attracts the nation's (indeed, the world's) best and brightest scientists and engineers to LLNL. Inspired by a sense of purpose and a high standard of excellence, LDRD-funded research often launches stellar careers, initiates strategic institutional collaborations, produces game-changing technical capabilities, and even forms the foundation entirely new fields of science. Empowered by the program, the impact our technical staff makes is often felt well beyond the DOE mission space.

It is no surprise then that every year, several of Livermore's LDRD principal investigators are recognized for the ground-breaking results of a project or for long-term contributions to their fields. The following short list of stories attests to the exceptional talents of these researchers and underscores the vitality of Livermore's LDRD program.

U.S. DEPARTMENT OF ENERGY | Office of Science

Project: A Short-Pulse, Laser-Driven Particle Beam Capability (17-ERD-039)

Principal investigator: Tammy Ma

LLNL plasma physicist **Tammy Ma** has been named a recipient of an award from the prestigious **DOE Office of Science Early Career Research Program** (ECRP). The program, now in its ninth year, is designed to bolster the nation's scientific workforce by providing support to exceptional researchers during their crucial early career years, when many scientists do their most formative work. Under the program, Ma will receive a total of $2,500,000 over five years for her proposal, "Multi-ps short-pulse laser-driven particle acceleration for novel HED and ICF applications."

"I am so grateful for everything the Lab has provided to allow me to thrive -- an incredibly nurturing environment, freedom and support to be innovative, the LDRD grant that laid the groundwork for this project, mentors that continuously encourage me, and the family of colleagues that makes it fun to come to work every day," Ma said. "I'm honored to receive this award, and the coolest part is that I'll get to extend the work of many of the LLNL giants that came before—this type of short-pulse particle acceleration was first discovered on the Nova laser, and now I get to use NIF ARC to push it forward into the multi-picosecond, high-energy regime."

Ma is an experimental plasma physicist in inertial confinement fusion and high energy density physics. She earned her bachelor's degree in aerospace engineering from Caltech in 2005 and received her master's degree in 2008 and Ph.D. in 2010, both from the University of California, San Diego. Following graduate school, she completed a postdoc at LLNL before becoming a staff scientist in 2012.

Ma currently serves as the leader of the X-Ray Analysis Group for LLNL's Inertial Confinement Fusion Program at the National Ignition Facility. Ma has authored or co-authored more than 140 peer-reviewed journal publications and has been recognized with the Stix Award for Outstanding Early Career Contributions to Plasma Research by the American Physical Society and the Presidential Early Career Award for Science and Engineering, the highest honor bestowed by the U.S. government on science and engineering professionals in the early stages of their independent research careers.

Awardees were selected from a large pool of university and national laboratory-based applicants. Selection was based on peer review by outside scientific experts.

Project: The New Frontier of Nuclear Science: Nuclear Reactions and Radiochemistry at the National Ignition Facility (16-SI-001)

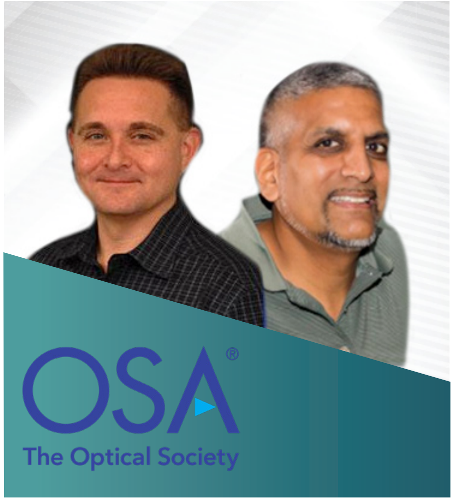
Principal investigator: Dawn Shaughnessy

The American Chemical Society (ACS) has named LLNL chemist **Dawn Shaughnessy** as a fellow. She is one of 51 fellows selected in 2018. The fellows program began in 2009 as a way to recognize and honor ACS members for outstanding achievements in and contributions to science, the profession, and ACS. "I am very honored that my colleagues in nuclear and radiochemistry nominated me for this fellowship," she said. "I truly enjoy working with them and the American Chemical Society in promoting nuclear chemistry to the next generation of scientists."

Shaughnessy is the group leader for experimental nuclear and radiochemistry and the principal investigator for the heavy element group at LLNL. Grounded in early research that was supported by LDRD, she and her colleagues co-discovered six new elements on the periodic table, the heaviest elements found to date. One of them—element 116, Livermorium—was named in honor of LLNL and the city of Livermore, California.

Shaughnessy was recently mentioned in an article in *Nature* magazine on contributions by women scientists to the discovery of elements and their properties ("Celebrate the Women Behind the Periodic Table," January 28, 2019). She was also inducted into the Alameda County Women's Hall of Fame in Science in 2011 and was awarded the inaugural LLNL Early and Mid-Career Recognition Award.

Founded in 1916, the **Optical Society of America** (OSA) is the leading professional association in optics and photonics, home to accomplished science, engineering and business leaders from all over the world. Fellow membership in OSA is limited to no more than 10 percent of the membership and is reserved for members who have served with distinction in the advancement of optics and photonics.



Project: Science of Finishing of Novel Optical Materials (17-ERD-005)

Principal investigators: Tayyab Suratwala

LLNL researcher **Tayyab Suratwala** has been named a fellow of the OSA. He was cited for "numerous, high-impact scientific and technological contributions improving optic technologies, specifically in the areas of optical fabrication and high laser damage resistant optics and coatings, enabling high-energy laser systems." He has spent more than 20 years at LLNL and currently serves as the program director for optics and materials science and technology. "I am truly honored to be elected as a fellow of OSA," Suratwala said. "I am fortunate and grateful for having the opportunity to work with such a great, talented LLNL team on challenging optic problems and novel optic technologies."

Project: Arbitrary Control and Characterization of Laser Waveforms and Interactions at Picosecond Resolution over Long Record Lengths (18-ERD-029)

Principal investigators: John Heebner and Ryan Muir

LLNL researcher **John Heebner** has also been elected a fellow of OSA and was cited for his "numerous innovations, achievements and technical leadership in high-energy laser systems and integrated optics including nonlinear optical microresonators and ultrafast light deflectors." Heebner, now the lead for the Ultrafast Optical and Electronics Systems Group, came to LLNL in 2003 and served as lead scientist for the front end of the National Ignition Facility laser system. He developed the chip-scale SLIDER deflector that set a world record for the fastest deflection of a light beam and recently designed the architecture for the high-contrast front end of the ARC Petawatt upgrade. Regarding the OSA announcement, Heebner said, "It's truly an honor to be elected a fellow of the Optical Society of America. It's humbling to be included among scientists and engineers I've looked up to as role models."

Project: Rapid Closed-Loop Control of Additive Manufacturing with Machine Learning (17-ERD-037)

Principal investigator: Brian Giera

Project: Optimal Fabrication Methodologies for Additive Manufacturing (14-ERD-087)

Principal investigator: Todd Weisgraber

DFG Deutsche Forschungsgemeinschaft

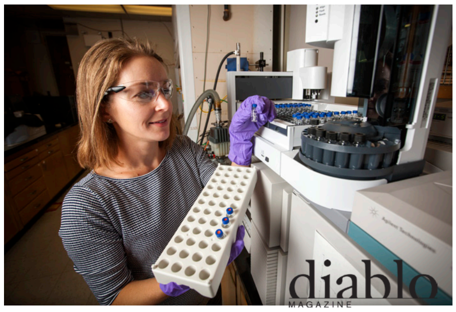
Using HPC resources at LLNL, the LDRD 14-ERD-087 team (Brian Giera, Luis Zepeda-Ruiz, Andrew Pascall, and PI Todd Weisgraber) developed a mesoscale model that reveals exquisite details of colloidal packing morphology and deposit crystallinity. While this work was originally intended to optimize LLNL's electrophoretic deposition (EPD) additive manufacturing technology, German researchers from University of Duisburg-Essen took notice and connected with **Brian Giera** at a conference in South Korea to learn how the model might help them develop coatings for their neural implants. With their help, Giera wrote a proposal and was awarded the **Mercator Fellowship**, by the Deutsche Forschungsgemeinschaft (DFG). Like its counterpart in the United States, the National Science Foundation, the DFG is the central, independent research funding organization in Germany, supported primarily by the German federal and state governments. The DFG awards Mercator Fellowships to encourage collaboration between researchers at domestic and foreign institutions. The award will fund 1–2 month trips to Germany over the next three years during which Giera will extend the model to help the researchers at Duisburg-Essen to use EPD to create thin and smooth neural implant coatings.

Three LDRD principal investigators, along with two other LLNL researchers, joined an eclectic group of entrepreneurs, writers, executives, philanthropists and more on *Diablo Magazine's* annual "40 Under 40" list, which recognizes young professionals in the East Bay who are leading the charge in their fields.

Project: Printed Biocatalysts for Natural Gas Upgrading (17-FS-027); A Design Platform for Electrochemical Conversion of Carbon Dioxide (18-ERD-010)

Principal investigator: Sarah Baker

Sarah Baker, a staff scientist and deputy group leader for the Functional Materials Synthesis and Integration Group, works on developing technologies to help mitigate climate change. Targeting more efficient ways to mitigate methane emissions (a potent greenhouse gas), she led a project to demonstrate that 3D printed enzymes (catalysts derived from micro-organisms) could directly convert methane to methanol. She also is leading a project to work toward industrial adoption of LLNL's carbon capture materials.



Sarah Baker named as one of Diablo Magazine's *"40 Under 40."*

Project: Optimizing Engineered Flow-Through Electrodes for Energy Applications (16-ERD-051)

Principal investigator: Marcus Worsley

Marcus Worsley, a chemist in the Advanced Materials Synthesis Group, aims to develop novel nanostructured and porous materials, such as aerogels and nanocomposites, for energy and environment-related applications, such as energy storage, gas sensing and catalysis.

Marcus Worsley named as one of Diablo Magazine's *"40 Under 40."*

His recent areas of research have focused on finding ways to use various additive manufacturing techniques, such as 3D printing, to overcome materials and device limitations in this field.

Leily Kiani named as one of Diablo Magazine's *"40 Under 40."*

Project: Efficient, High-Power Mid-Infrared Laser for National Security and Scientific Applications (16-ERD-021)

Principal investigator: Leily Kiani

Leily Kiani, a postdoctoral researcher in the Fiber Technologies Group, explores extending the utility of fiber lasers by increasing the frequency ranges accessible to fiber-based systems through novel fiber development and nonlinear frequency conversion. A recent focus of her work has been to investigate the ultimate noise performance in short pulse fiber amplifiers, with important implications for laser-driven particle accelerators and for realizing previously unobtainable states of matter through interaction with high intensity laser pulses.

LLNL LDRD scientists discovered that at the thermodynamic conditions of the Earth's core, metals such as iron and nickel become electronegative and attract electrons, and noble gases, which normally show very little interactivity, react with metals. This research affords the first opportunity to validate models of high-compression/low-strain-rate frictional heating and shear-induced chemistry and physics, one application of which might be the characterization of the safety of weapon system components subjected to high-compression/low-strain-rate insults (18-LW-036). (Image by Adam Connell)

LDRD on Journal Covers (*and TV*)

The impact of LDRD research extends beyond the DOE mission space into the wider scientific arena. Evidence of this can be seen in is seen in both the number of scientific journal articles and front-cover features in high-visibility journals documenting LDRD project results. In FY18, LDRD-funded research was even featured on television.

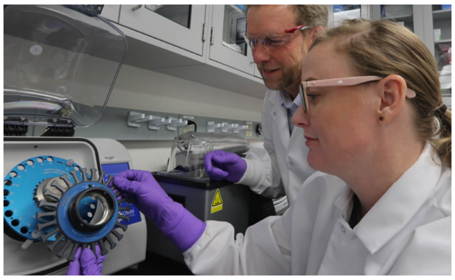
Project: Physical States and Processes in Inertial-Confinement Fusion: Matter at Extreme Energy Density (14-SI-003)

Principal investigator: Gilbert Collins

Horizon, BBC's longest running science program, visited LLNL to film segments for "Horizon: Journey into Jupiter," a co-production with the Discovery Science Channel. In October, 2017, they visited the National Ignition Facility to film and interview scientists Marius Millot, Jon Eggert, Dayne Fratanduono, and Peter Celliers about their discovery science experiments on liquid metallic hydrogen—research that was supported in part by LDRD. They also interviewed scientist Thomas Kruijer about his work relating to the age of Jupiter and filmed relevant meteorite samples in his laboratories. The episode aired on January 24, 2019.

Project: Forensic Science of Genetically Variant Peptides (16-SI-002)

Principal investigator: Bradley Hart



CH7 NEWS

LLNL scientists Katelyn Mason and Deon Anex prepare to pulverize forensic bone samples prior to demineralization and extraction of proteins to find identity markers. (Photo by Julie Russell/LLNL.)

On May 22, 2018, Tim Didion, a reporter with *ABC7 News*, visited the Forensic Science Center to interview LLNL's Katelyn Mason and Deon Anex regarding a new method for individual identification using protein identity markers found in human bones (see "Research Highlights"). The segment aired on the evening news on May 23. The new protein marker technology addresses a 2009 National Research Council report on forensic science that detailed the weaknesses of many current approaches and reported an urgent need for new science-based forensic methods. While DNA-based forensics remains the first choice for human identification, the new protein marker technology provides an alternative when DNA has been destroyed by time or extreme conditions.

Project: Rapid Synthesis, Functionalization, and Assembly of Nanometer-Scale Particles for Designer Materials (13-ERD-022)

Principal investigator: Thomas Han

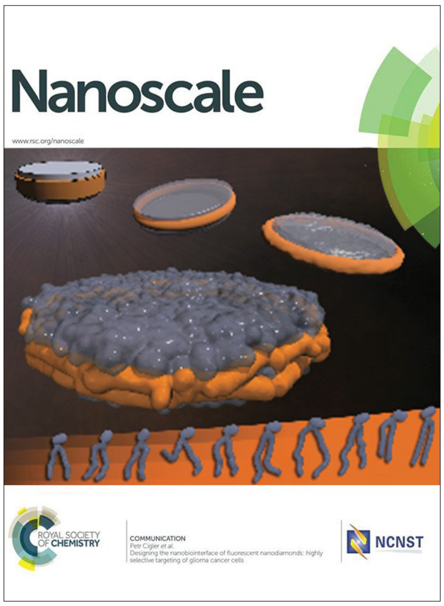
Project: Deterministic Multifunctional Materials and Manufacturing Initiative (14-SI-004)

Principal investigator: Christopher Spadaccini

Project: Materials Informatics for Synthesis, Optimization and Scale-Up of Functional Materials (16-ERD-019)

Principal investigator: Thomas Han

Metal foams (or porous metals) represent a new class of materials with a unique combination of properties including light weight, high surface area, high electrical conductivity, and low thermal conductivity that can advance technologies in electronics, thermal insulation, sensing, catalysis, and energy storage. Livermore researchers have fabricated ultralight silver foams (silver aerogels) with predictable densities down to single-digit mg/cm^3. The team prepared high-purity silver nanowires by polyol synthesis, purified them through selective precipitation, and suspended them in water for subsequent freeze-casting and freeze-drying to enable the formation of aerogels. Silver aerogels prepared in this method have unique anisotropic microporous structures, with density precisely controlled by nanowire concentration down to 4.8 mg/cm3. The research has applications to stockpile stewardship, laser target development, and energy and resource security. It was featured as the journal cover in the December 2017 issue of *Nano Letters*.



Graphic by Timothy S. Carpenter.

Project: Nanometer-Scale Particle Platform for Drug Delivery to the Brain (15-LW-023); Nanometer-Scale, Particle-Based Immunotherapy for Cancer Treatment (17-LW-051)

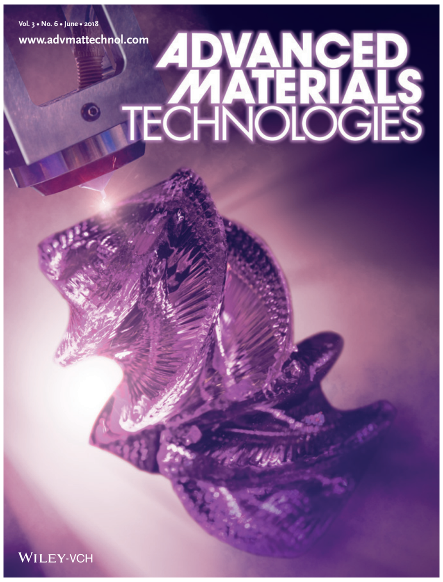
Principal investigator: Sean Gilmore

Nanoparticles are nanoscale objects, typically 1-100 nanometers in size, that can be used for a variety of purposes, including formulating medicines or vaccines. For several years, LLNL has been developing a novel class of nanoparticles for biomedical applications that are highly biocompatible and offer advantages that other nanoparticle types do not. These nanolipoprotein particles (NLPs), consist of a phospholipid bilayer stabilized by an apolipoprotein scaffold protein and are lab-made versions of HDL or "good cholesterol" that are used by the body to transport cholesterol and triglycerides in the blood. While preliminary studies had previously demonstrated that the type of phospholipid used to synthesize these particles can affect their stability, it was unclear how specific phospholipid features impact the nanoparticle stability under physiologically relevant condition. An LLNL team recently conducted a thorough assessment of how phospholipid structure impacts stability of biomimetic nanoparticles

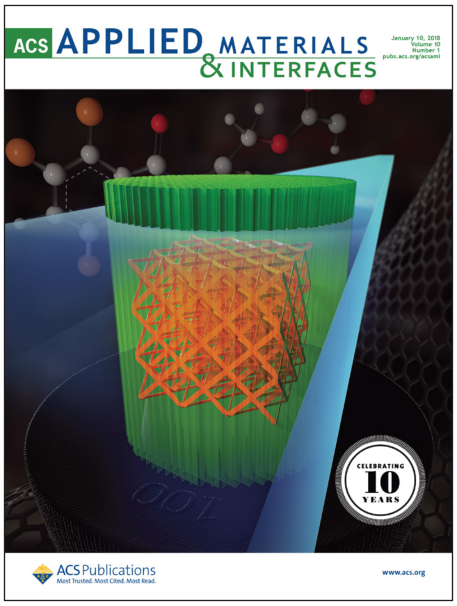
in blood serum at 37° C, closely mimicking the environment and conditions the particles would encounter circulating in the blood stream. This key information has important implications for using these NLPs in vivo and provides insight into how to tune the particle stability for applications ranging from diagnostics to drug delivery. This study assessed the stability of NLPs with varying lipid compositions in blood serum. The results, published as the inside-front-cover feature article in the April 2018 issue of *Nanoscale*, provide a foundation for subsequent optimization of NLP composition to tailor the stability for particular in vivo applications. This research leverages and strengthens LLNL's nanoscale bioengineering capabilities to advance a cure for one of the world's most widespread and deadly diseases.

Project: Fabrication of Functionally Graded Optical Components Using Additive Manufacturing (16-SI-003)

Principal investigator: Rebecca Dylla-Spears



In an article featured on the back cover of the January 28 issue of *Advanced Materials* Technologies, a team of researchers described a method for fabricating optical quality silica and silica–titania glasses using three-dimensional (3D) printing. Key to this success was the combination of sol–gel derived silica and silica–titania colloidal feedstocks, direct ink writing (DIW) technology, and conventional glass thermal processing methods. Printable silica and silica–titania sol inks are prepared directly from molecular precursors by a simple one-pot method, which is optimized to yield viscous, shear-thinning colloidal suspensions with tuned rheology ideal for DIW. After printing, the parts are dried and sintered under optimized thermal conditions to ensure complete organic removal and uniform densification without crystallization. Characterizations of the 3D-printed pure silica and silica–titania glasses show that they are equivalent to commercial optical fused silica and silica–titania glasses. More specifically, they exhibit comparable chemical composition, SiO2 network structure, refractive index, dispersion, optical transmission, and coefficient of thermal expansion. 3D-printed silica and silica–titania glasses also exhibit comparable polished surface roughness and meet refractive index homogeneity standards within range of commercial optical grade glasses. This method establishes 3D printing as a viable tool to create optical glasses with compositional and geometric configurations that are inaccessible by conventional optical fabrication methods. This research has a range of applications across the DOE and NNSA mission space, including laser technologies and space-based optics.



Project: Accelerated Development of Multiscale Materials (15-ERD-019)

Principal investigator: Juergen Biener

Two-photon lithography (TPL) is a high-resolution additive manufacturing (AM) technique capable of producing arbitrarily complex three-dimensional (3D) microstructures with features 2 to 3 orders of magnitude finer than human hair. This process finds numerous applications as a direct route toward the fabrication of novel optical and mechanical metamaterials, miniaturized optics, microfluidics, biological scaffolds, and various other intricate 3D parts.

As TPL matures, metrology and inspection become a crucial step in the manufacturing process to ensure that the geometric form of the end product meets design specifications. X-ray-based computed tomography (CT) is a nondestructive technique that can provide this inspection capability for the evaluation of complex internal 3D structure. However, polymeric photoresists commonly used for TPL, as well as other forms of stereolithography, poorly attenuate x rays due to the low atomic number (*Z*) of their constituent elements and therefore appear relatively transparent during imaging.

To address this issue, researchers have developed optically clear yet radiopaque photoresists for enhanced contrast under x-ray CT. As reported in the cover article of the January 10, 2018 issue of *Applied Materials & Interfaces*, this new AM feedstock increases x-ray attenuation by a factor of more than 10 times while preserving the resolution of parts produced on the millimeter scale with sub-150-nm features. This formulation is expected to play a critical role in enabling fabrication of functional polymer parts to tight design tolerances for application across the DOE and NNSA mission space.

Project: Deterministic Multifunctional Materials and Manufacturing Initiative (14-SI-004)

Principal investigator: Christopher Spadaccini

As described in the cover article of the December 2018 issue of *Science Advances,* a team of researchers have introduced a new class of metamaterials that can nearly instantly respond and stiffen 3D-printed structures when exposed to a magnetic field, a development that could be applied to next-generation helmets, wearable armor, and a host of other innovations. These "field-responsive mechanical metamaterials" (FRMMs) employ a viscous, magnetically responsive fluid that is manually injected into the hollow struts and beams of 3D-printed lattices. Unlike other shape morphing or so-called "4D-printed" materials (the fourth dimension being time), the overall structure of the FRMMs does not change. The fluid's ferromagnetic particles located in the core of the beams form chains in response to the magnetic field, which stiffens the fluid and the lattice structure as a result. This response happens rapidly—in less than a second.

The Long-Term Impacts of LDRD Investments: Centers for Strategic Partnerships

Sometimes it's easy to predict from a project's description what the impact of the research will be, and the "Awards" and "Journal Covers" sections of this overview provide some follow-up by illustrating how LDRD research has actually been received by the scientific community and the media. Arguably, the more interesting though less often told stories are about the long-term impacts of LDRD research, be it a single project or the sustained investment in a topic over time.

The two stories below each shine a light on the value of sustained investment in a nascent or burgeoning field. In both cases, LDRD investment began with a broad vision of how building LLNL's capabilities in a new area of science and technology could be of strategic use in better achieving national missions. Driven by a spirit of innovation, scientists and engineers delivered basic science discoveries and developed next generation mission solutions. In both stories, as is often the case, sustained investment led to more than just technological breakthroughs; it led to a body of knowledge that laid the groundwork for new mission-focused capabilities that further evolved into centers for external collaborations.

LDRD Investments Lead to an "Open Campus" Advanced Manufacturing Laboratory

Advanced manufacturing—a field that incorporates novel materials, additive manufacturing, and high-performance computing (for design models, simulations, characterization, and more)—is an area of rapid growth in industry, fueling the development of innovative products from customized medical implants to high-performance car parts and more. Advanced manufacturing

LLNL's new Advanced Manufacturing Laboratory accelerates manufacturing technology development through strategic partnerships with industry and academia.

is also a new tool for meeting NNSA missions in national security, energy security, and perhaps most critically, stockpile stewardship. Beginning in 2012, LDRD funded a body of research that formed the foundation of an entirely new capability, including numerous patents for novel materials, tools, and manufacturing processes. It's impact on mission? "We're already seeing significant decreases in manufacturing cost and footprint, improved flexibility, and products and components that are vastly superior to those obtained through traditional manufacturing," said Engineering Associate Director Anantha Krishnan.

Early support from LDRD gave the Laboratory a leading edge in this rapidly evolving field, one way to maintain that edge is to learn from others, specifically with regard to transferring this technology to industry. Toward that end, in the summer of 2018, LLNL opened the Advanced Manufacturing Laboratory (AML), a $10 million, 14,000-square-foot facility located in the **Livermore Valley Open Campus** (LVOC), a cluster of buildings just beyond the borders of LLNL that are designed to facilitate collaborations with academic and industry partners. This first-of-its-kind facility features a large wet lab where three-dimensional printing, materials research, chemical work, carbon capture technology, and other research activities can be performed. A 5,000-square-foot dry lab houses industrial-size manufacturing machines, including laser powder bed fusion and diode-based metal additive manufacturing systems, with space for metrology and characterization as well.

According to Chris Spadaccini, LLNL's Director of the Additive Manufacturing Initiative and an early LDRD researcher in the field, the AML is a result of the Laboratory's desire to improve responsiveness and learn from external partners by actively pursuing collaborations with industry and academia that could benefit both parties. "We're looking for equal investors and complementary "spin in/spin out" projects where we can help companies and vice versa….It's not a pay-to-play facility. We hope and expect that this will accelerate development of advanced manufacturing technology that will benefit both our external partners and our internal programs. We expect students and postdocs to be here and see this as a recruiting pipeline as well. We hope our partners will help guide AML's future, and we want to learn as much from them as they do from us."

LDRD Investments Lead to a Data Science Institute

Machine learning. Deep learning. Artificial intelligence. Computer vision. Big data analytics.

These aren't just techie buzzwords—they're all areas of research that fall under the sweeping term "data science," a field that underpins some of the most powerful antiterrorist and antiproliferation tools currently under development at LLNL.

Launched earlier this year, the Data Science Institute (DSI) is an organization designed to bring together myriad topics considered "data science" under one umbrella, establishing a centralized hub for education, collaboration, and the building of a workforce pipeline that targets soon-to-be college graduates. The DSI, which includes over 150 data scientists at the Laboratory, was built, in large part, on a body of research sustained by LDRD since 2012.

Peer-Timo Bremer, a member of the Data Science Council, explained that because data science is so "cross-cutting" and difficult to define, the DSI was a necessary step, not just for the benefit of Laboratory scientists, but for those outside the gates as well. He pointed to large-scale collaborative projects such as ATOM (Accelerating Therapeutic Opportunities in Medicine), which seeks to use machine learning and data analytics to enhance precision medicine and speed up drug development in response to biothreats, and the ADAPD (Advanced Data Analytics for Proliferation Detection) projects, aimed at developing advanced machine learning algorithms to help detect nuclear proliferation indicators earlier, more thoroughly, and more robustly than ever before. The algorithms will combine cues from multiple sensor measurements to detect patterns too subtle or too noisy to be detected from any one sensor alone.

According to DSI Director Mike Goldman, other ongoing projects apply data science to research in materials science using machine learning to predict performance, cognitive simulation for stockpile stewardship, basic science, advanced manufacturing, and energy and climate security. "The problems we work on here are unique and challenging and difficult, and we use data you're not going to see anywhere else," Goldman added. "Also, you've got the computing power here to utilize that data."

United States Department of Energy

NNSA
National Nuclear Security Administration

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LDRD
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