Lawrence Livermore National Laboratory

Science & Technology REVIEW

January/February 2023

RISKS AND REWARDS OF DISRUPTIVE RESEARCH

Also in this issue:

About the Cover

The vortex on this issue’s cover represents the sense of uncertainty experienced by scientists in the initial stages of exploring a new research path. The article beginning on p. 4 introduces research projects of higher technical risk conducted under Lawrence Livermore’s Disruptive Research (DR) Program, a component of the Laboratory Directed Research and Development Program. If successful, DR projects yield order-of-magnitude rewards. If DR projects fail to meet stated goals, they offer different rewards by shaping future research and investments.

Cover design: Mark Gartland

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation’s security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory’s scientific and technological accomplishments in fulfilling its primary missions. The publication’s goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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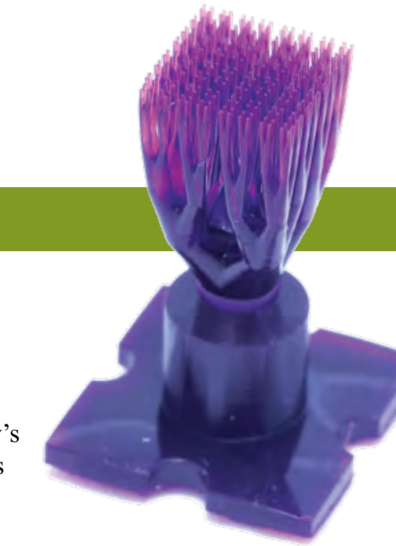


Feature

R&D100 Winners

R&D 100 AWARDS 60TH ANNIVERSARY 2022

Departments

Earth System Science Network Upgrades

Lawrence Livermore, Oak Ridge, and Argonne national laboratories have completed the first major step in upgrading the Earth System Grid Federation (ESGF) network, the international data infrastructure that links climate modeling centers and enables researchers to archive and share climate model output data. Increasingly large data sets, generated at the terabyte and petabyte level, necessitate updated data management approaches and faster download of data subsets. Modernizing the global data system will better support scientists working on the World Climate Research Programme's Coupled Model Intercomparison Project.

In the past, ESGF replicated data only to Livermore, its principal compute node. To lay the groundwork for an ESGF2, the three laboratories began a dual backup of 8 petabytes (10^{15} bytes) of Livermore-hosted climate data to nodes at Argonne and Oak Ridge. With a more broadly distributed architecture, ESGF2 can support faster, more secure, and more easily scalable computing and collaboration. "The upgrades enable easier and faster data access so users better understand what climate will look like in the future," says Sasha Ames, Lawrence Livermore's lead for ESGF2.

ESGF2 will feature data livestreaming and server-side computing capabilities and may also host observational data from NASA and the National Oceanic and Atmospheric Administration. Livermore scientists earned a 2017 R&D 100 Award for developing ESGF (see *S&TR*, April/May 2018, pp. 16–17) and served as the network's initial lead.

Contact: Sasha Ames (925) 424-4644 (ames4@llnl.gov).

New Alloy for Cheaper Catalysis

Catalysts for hydrogenation processes used in the flavoring and fragrance industries and in converting biomass to valuable chemicals typically rely on costly precious metals. Lawrence Livermore scientists and collaborators have demonstrated an effective and more affordable hydrogenation catalyst composed of earth-abundant materials. Published in the September 21, 2022, issue of the *Journal of the American Chemical Society*, the research presents the principle that a more reactive metal can initiate the catalytic process.

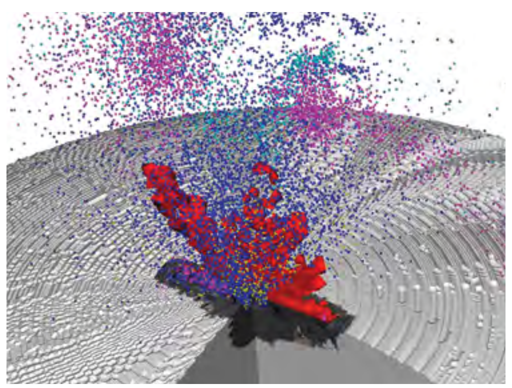
The new method involves fabricating diluted alloys of nanoporous copper (NPC) doped with titanium to successfully dissociate hydrogen atom pairs, a vital chemical reaction for hydrogenation. The study found that NPC doped with small amounts of titanium enables hydrogen–deuterium exchange at rates five to seven times higher than with undoped NPC. Experimental findings, supported by model analysis, indicate that isolated titanium atoms on the copper surface enable catalysis by acting as sites for hydrogen–deuterium recombination instead of dissociative adsorption of hydrogen, a more stringent, rate-limiting step.

The research may apply to other cost-effective compositions of hydrogenation catalysts as well. "This approach is of broad interest and significance because it looks at a new alloy composition with potential for selective hydrogenation catalysis," says Laboratory materials scientist Juergen Biener, one of the study's co-authors. "Our work creates opportunities to expand dilute alloy catalyst design to include early transition metals for hydrogenation reactions."

Contact: Juergen Biener (925) 422-9081 (biener2@llnl.gov).

The Right Stuff for Dimorphos

Detailed guidelines for interpreting experimental data gathered in the September 2022 collision of NASA's Double Asteroid Redirection Test (DART) spacecraft with the asteroid Dimorphos were available in advance of NASA's asteroid-deflection test thanks to impact simulations by Lawrence Livermore researchers. Led by Kathryn Kumamoto, a Livermore team ran more than 300 separate 3D impact simulations in which the Laboratory's Spheral hydrodynamics code sampled more than seven different material parameters of the asteroid, including shape, mass, elasticity, and structure. Machine-learning algorithms selected parameter combinations to efficiently cover the study's search space. The results, published in the October 2022 issue of *Planetary Science Journal*, predicted properties of asteroid material that could result from a DART-like kinetic impact.



MIKE OWEN

Many simulation results matched predictions from a separate model calculating velocity change from the DART impact, while conclusions about parameters such as the effect of porosity on an asteroid's post-impact change in velocity and the volume of resulting ejecta varied. However, the simulations offer impact modelers opportunities to infer properties of the asteroid Dimorphos along with photographs from DART's camera and the change-in-velocity result. "This initial study is an important step for explicitly describing what we can and cannot predict about impacting an uncharacterized asteroid," says Kumamoto. Data gathered from Dimorphos's DART-created impact crater, its companion asteroid Didymos, and a future European Space Agency mission are expected to narrow the range of Dimorphos's possible material qualities.

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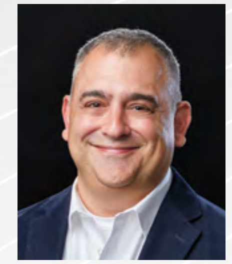

A Legacy of Innovation

LAWRENCE Livermore National Laboratory takes pride in being known as the "new ideas" laboratory, a tagline reflecting the earliest aspirations of its founders. For more than 70 years, Livermore staff have thought outside the box to keep the nation and world secure. Yet, even within such an innovative environment, aversion to risk creeps in and restrains powerful and transformative ideas. Fear of failure and the ramifications of unachieved goals exert influence. Rather than embrace risk to achieve great benefit, staff hesitate to drive disruptive research. However, with vastly more capable experimental and computational tools arriving year after year to accelerate the Laboratory's mission, Livermore is ripe for more risk-taking research to achieve high-reward advances in science and technology.

Venture capitalists in the private sector and government organizations such as the Defense Advanced Research Projects Agency (DARPA) foster a risk-taking culture in research and development. Their high-risk–high-reward outlook requires a high tolerance for failure. That outlook has cleared the path for groundbreaking advances such as the internet, GPS, drones, and the creation of technology giants in California's Silicon Valley.

In 2019, Lawrence Livermore set out to inject a similar spirit of risk-taking into its Laboratory Directed Research and Development (LDRD) Program by initiating the LDRD Disruptive Research (DR) pilot program. All LDRD Program projects carry inherent risk of failure. Many, however, are designed to achieve important, yet incremental, advances rather than revolutionary breakthroughs. Principal investigators often incorporate risk mitigation and engage peers in proposal review. In contrast, the DR Program intentionally selected only high-risk–high-reward ideas and subsequently manages them toward aggressive goals and project-end criteria.

The feature article describes a curated selection of DR Program projects. In one project, a team fabricated and tested a new cooling concept for hypersonic vehicles that utilizes additive manufacturing of ultra-high-temperature materials and a multiscale internal architecture for transpiration cooling. By pairing ultracapacitors with a unique laser gain media, another highlighted project demonstrated 120 joules of output energy and could ultimately lead to bench-sized laser configurations rather than building-sized facilities. The first DR project tranche also included an attempt to develop a new optoelectronic device that, if successful, could have increased data transfer rates to satellites by orders of magnitude.

Representing the latest instantiation of the DR Program are two projects brimming with exciting innovation activities. One team works toward developing an iron redox flow battery technology with the potential to provide inexpensive, durable, large-scale energy storage for the electrical grid. In another similarly disruptive and newly funded project, researchers seek to revolutionize industrial fertilizer manufacturing and utilization to radically reduce the massive carbon output of current practices. Projects in the DR category have, overall, shown significant successes.

Continuing the thread of bold innovation and outcomes, a series of research highlights describes the Laboratory's three 2022 R&D 100 Award winners and one past winner. Each year, *R&D World* magazine recognizes its top 100 new technologies with an R&D 100 Award. Livermore's 2022 award recipients developed a direct ink writing process to 3D-print complex optical-quality glass objects, invented feedstock materials with functional properties for additively manufacturing energy storage and other devices, and designed gratings to tolerate the petawatt-level laser operations required for new discoveries in astrophysics and quantum physics, among other fields. Winning a 2013 R&D 100 Award set one Laboratory technology—DNATrax—onto a commercial path starting with ensuring safety from hazardous indoor air conditions to its current application by the company SafeTraces for indoor air quality improvements.

None of the innovations presented in this issue of *Science & Technology Review* would exist in an institution operating with only an eye to the past. The Laboratory's goal is to foster the culture of risk-taking demonstrated by DR Program projects and new, award-winning technologies. Spreading a high-risk–high-reward outlook to other categories in the LDRD Program portfolio and throughout the Laboratory will ultimately catalyze the next generation of great Lawrence Livermore breakthroughs.

■ Chris Spadaccini is the Materials Engineering Division Leader.

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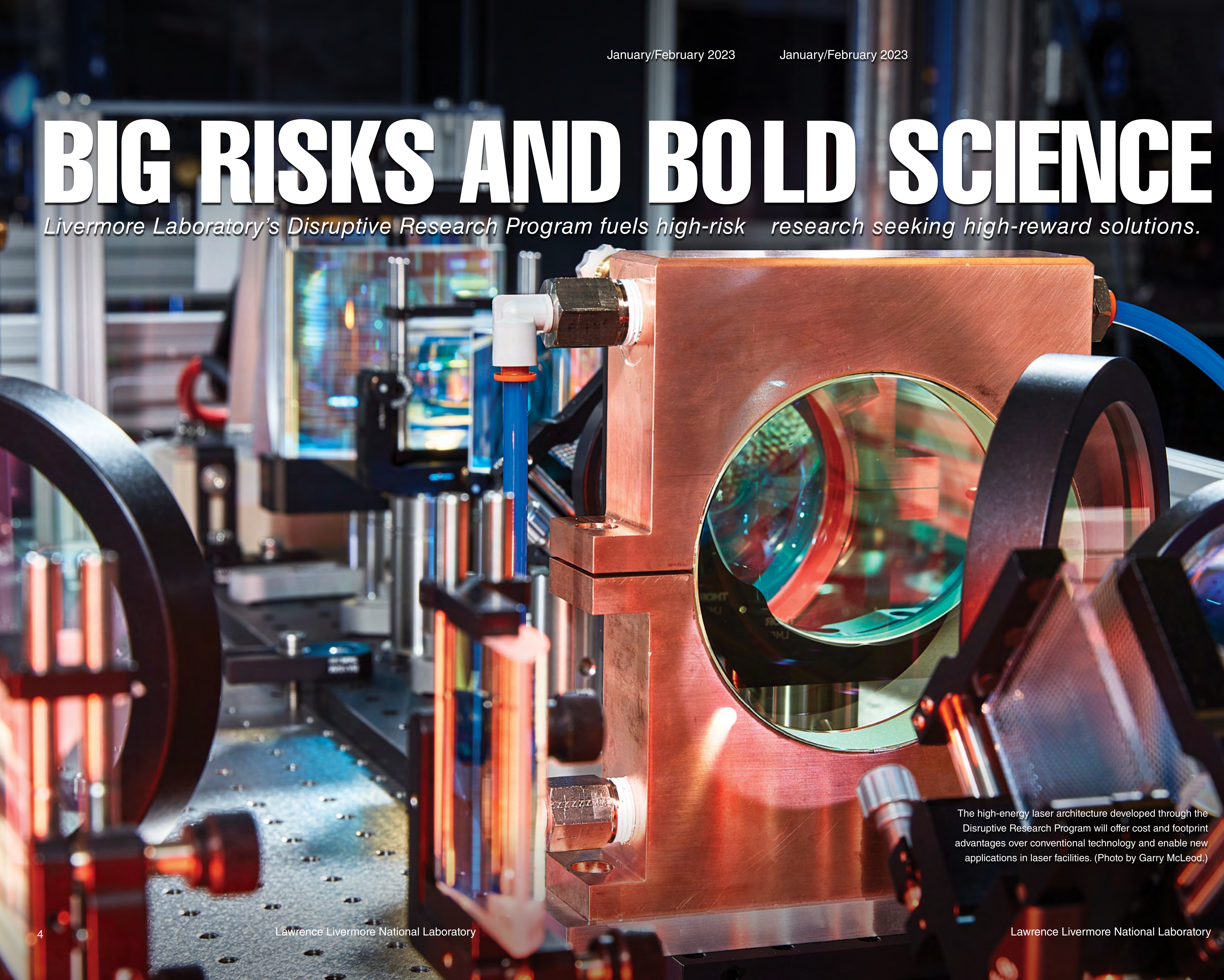
BIG RISKS AND BOLD SCIENCE

Livermore Laboratory's Disruptive Research Program fuels high-risk research seeking high-reward solutions.



The high-energy laser architecture developed through the Disruptive Research Program will offer cost and footprint advantages over conventional technology and enable new applications in laser facilities. (Photo by Garry McLeod.)

EVER evolving as a "new ideas" laboratory, Lawrence Livermore exemplifies bold scientific research through its Laboratory Directed Research and Development (LDRD) Disruptive Research (DR) Program. Launched in 2019, the Laboratory's DR Program supports research and development activities that are unconventional, innovative, and at the forefront of their fields. Livermore researchers are encouraged to embrace high levels of technical risk to yield transformative scientific advances, even if their projects ultimately fail. Successful DR project outcomes advance research by producing order-of-magnitude improvements, opening new program spaces, or creating positive impacts in Laboratory initiatives.

Now in its second funding cycle, the DR Program has achieved a shift in risk acceptance at Lawrence Livermore. With the first cycle of nine selected projects (see *S&TR*, August 2021, pp. 20–23) coming to a close and the second cycle approaching initial go–no-go milestones, the Laboratory will evaluate discoveries made and early successes, review lessons learned and occasional setbacks, and then forge next steps. The following representative projects from both funding cycles demonstrate how Livermore is carving a path in disruptive scientific research.

Laser-Focused on Innovation

In recent years, the Department of Energy (DOE) has designated high-intensity, ultrafast laser research as a key priority for national security and economic growth. Home to the National Ignition Facility (NIF), Jupiter Laser Facility, and some of the world's most renowned experts in laser research, Lawrence Livermore is well positioned to meet DOE priorities. Under the 2019 DR Program, Thomas Spinka, Program Element Leader for Laser Development in Livermore's Advanced Photon Technologies program, developed a revolutionary high-energy laser architecture that could open the door

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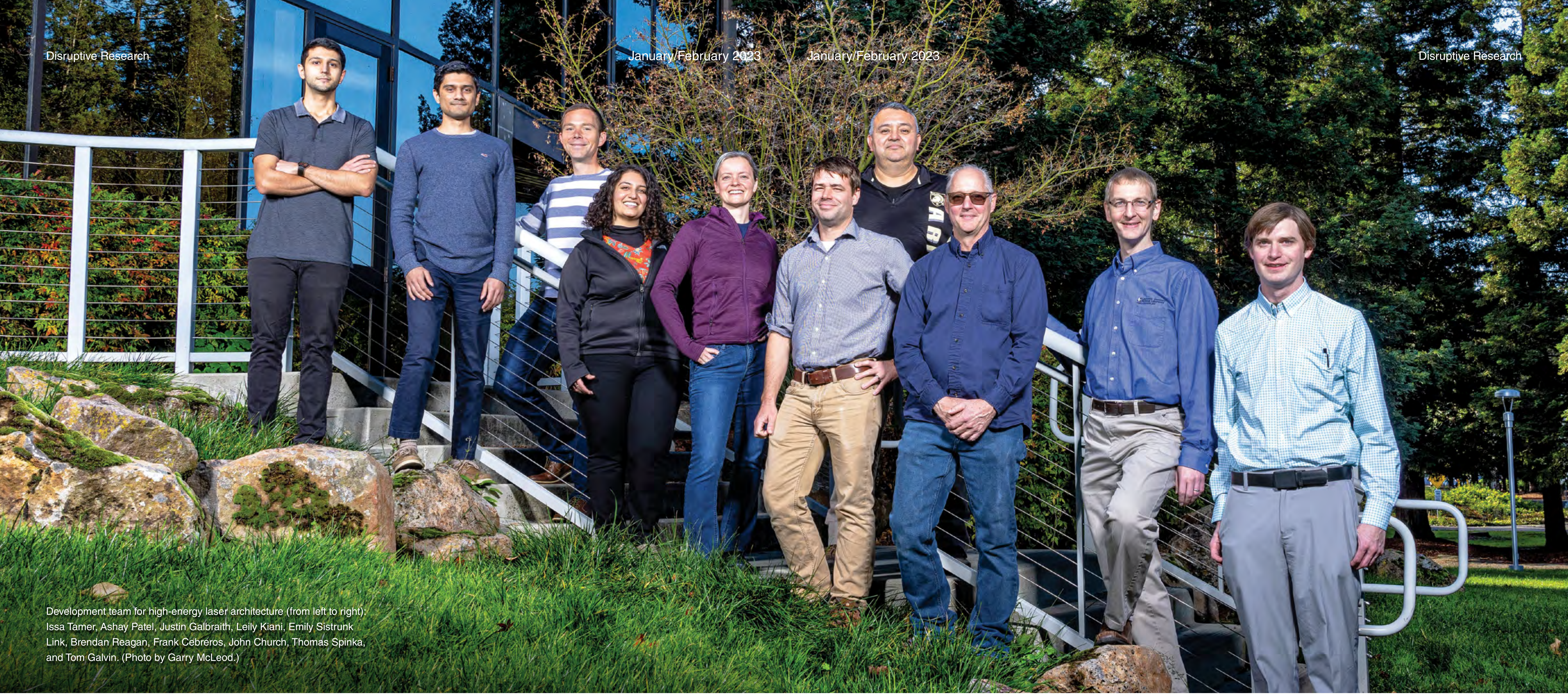

Development team for high-energy laser architecture (from left to right): Issa Tamer, Ashay Patel, Justin Galbraith, Leily Kiani, Emily Sistrunk Link, Brendan Reagan, Frank Cebreros, John Church, Thomas Spinka, and Tom Galvin. (Photo by Garry McLeod.)

for expanding laser research resources and serve as an alternative to current laser facilities.

Spinka and his multidisciplinary team of scientists and engineers combined a previously known but underutilized laser material with laser diodes and new capacitor technology that more effectively stores and releases electrical energy to meet the significant goal of reaching a 100-joule output by the end of the project. The team used yttrium-lithium-fluoride (YLF) crystals doped with thulium ions (Tm:YLF) as the laser's gain medium. Thulium ions in a YLF crystal lattice can store photons created in the pump laser diodes nearly 50 times longer than more traditional laser gain materials. The next component of this innovation called for pairing Tm:YLF crystals with ultracapacitors, which store electrical energy much more densely and less expensively than traditional electrolytic capacitors. Ultracapacitors cannot be paired with conventional laser materials that lack the ability to release their stored electrical energy rapidly enough.

In the project's first stage, the team combined ultracapacitors and laser diodes for the first time and demonstrated that the photons produced exhibited the right characteristics for pumping Tm:YLF laser crystals. The second stage proved that the pump photons could be stored efficiently in the laser crystal. Once these concepts had been proven, Spinka and his team needed to effectively extract the energy stored in the Tm:YLF crystal. "We initially targeted 10 joules as a goal, but we were fairly certain we could exceed that target," says Spinka. "Our stretch goal was 100 joules. When we achieved 120 joules, we were thrilled at the opportunities ahead of us and others in the field."

Regarding the impact of this project, Spinka explains, "Only a handful of laser materials have demonstrated 100-joule output over the past 60 years. Adding another material to that group at this stage is incredibly exciting." The outcomes of this project could lead to the development and use of smaller, lighter, more portable, and more cost effective high-energy lasers—a key step for growing a U.S. laser research base. Kilojoule-class lasers are immense and offer limited access to experimental teams. The Tm:YLF high-energy laser Spinka and his team developed under the DR Program shows tremendous promise in storing large amounts of energy in a space small enough to fit on one optical table rather than an entire room. Additionally, the success of Tm:YLF in Spinka's research may enable new secondary source applications, including nondestructive evaluation with x rays and muons (subatomic particles). The team is also testing ultrashort pulse laser capabilities (pulses mere femtoseconds in duration) and the thermal properties of the Tm:YLF gain material to better understand its operational limits.

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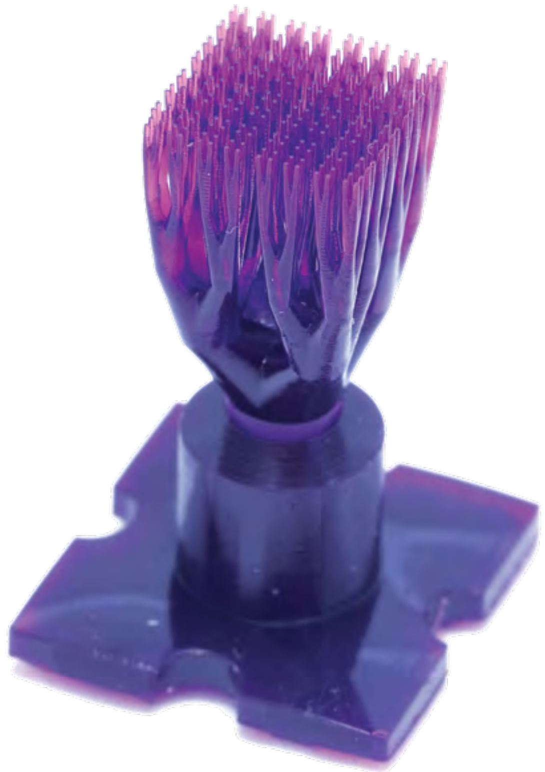


The additively manufactured vasculature structure (above) used for cooling hypersonic flight vehicles houses gold, which melts as the temperature of the vehicle's leading edge reaches 1,000°C. The increasingly narrow capillaries channel the molten gold in a predictably directed manner to effectively wet the ceramic and cool the flight vehicle. (Photo by James Cahill.)

Development team for thermal protection technology (from left to right): James Cahill, Bruce Yang, Swetha Chandrasekaran, Leila Sun, Josh Kuntz, Ellie Sobalvarro, Jesus Rivera, Wyatt Du Frane, Logan Bekker, and Bella King. (Photo by Garry McLeod.)

Keeping Cool at Mach Speeds

Structural integrity is a critical parameter in flight vehicles, especially those that reach hypersonic speeds (defined as Mach 5 or higher). At these velocities, a vehicle's leading edge can reach 3,000°C due to shock waves at the tip and friction along the surface. Such intense heat is well above the melting temperatures of most materials, presenting a major technical hurdle for hypersonic flight. Lawrence Livermore's James Cahill used his 2019 LDRD DR funding to additively manufacture a thermal protection system for hypersonic vehicles that could be a game changer for the field.

The foundation of Cahill's concept is metal transpiration cooling, in which heat is carried away from a material via liquid evaporation. He and his research team created a vascular structure that houses solid metal intended to melt and vaporize through the structure's branching tubes. "The process is similar to the way organisms cool their bodies through sweating," says Cahill. "In our concept, we found substantial cooling potential from both the melting and vaporization of the solid metal," says Cahill. The structure's dendritic channels extend outward, then narrow to increase capillary pressure and wick the melted metal toward the surface.

To proceed, the team needed to identify a robust material for the vasculature shell as well as an appropriate metal to melt within the structure. High-temperature ceramics, which have ideal properties including high melting points and strength at elevated temperatures, showed the most promise for the structure's exterior. The metal interior required a melting point of approximately 1,000°C to wet the ceramic shell, yet not oxidize, which would introduce additional phases and thermodynamics and complicate the cooling process. "We narrowed the choice down to silver and gold," says Cahill. "As noble metals, they are difficult to oxidize, and their melting temperatures are both in the right range. Gold happens to wet the ceramic much better than silver, so it was the ideal candidate to test our concept without adding too many other factors."

Cahill's team then manufactured the vasculature structure to test the concept. They fabricated an intricate ceramic structure with some sections no more than 100 to 200 micrometers wide. They began by printing a sacrificial polymer mold of the vasculature. Then, they used a refined casting process to create a ceramic slurry, similar in consistency to modeling clay, to infiltrate into the polymer mold. Once the ceramic was dried and set, they carefully burned out the polymer mold.

Following the components' manufacturing, Cahill's team faced a decisive milestone in the DR funding scheme to determine whether the metal transpiration cooling concept was effective. "If the structure didn't work, that was pretty much it for the project," says Cahill. Working with components only 1 to 2 centimeters in size, Cahill interrogated samples using a torch to simulate the necessary thermal gradients and high temperatures experienced in hypersonic flight. The data showed both melting and vaporization of the gold along with a significant 200°C drop in sample temperature. With this favorable result, Cahill now anticipates working to achieve scalability of manufacturing, technology transfer, and eventually real-world applications.

Development team for the tunable amplifier (from left to right): Saptarshi Mukherjee, Lars Voss, Sara Harrison, Laura Leos, and Soroush Ghandiparsi. (Photo by Garry McLeod.)

As Fast as a CHEETAh

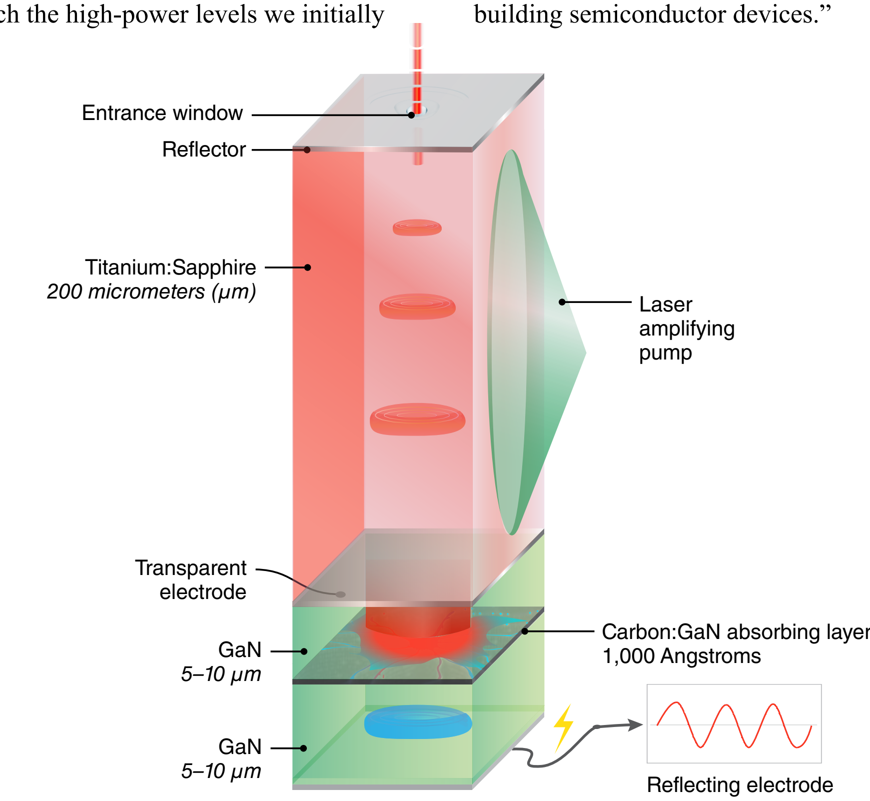
Optoelectronic devices are found in many everyday items, including fiber optic cables, satellite communications, LED lights, solar cells, and photodiodes. Designing and implementing advanced optoelectronic technology that is orders of magnitude faster and operates at much higher voltages is a national security focus area that comes with many challenges. Lars Voss, an engineering group leader, led a DR project to develop a laser-driven semiconductor that could theoretically operate at higher speeds and higher voltages than existing photoconductive devices, which could enable next-generation satellite communication systems capable of transferring more data at a faster rate and over longer distances.

The Compact High Efficiency Electrically Tunable Amplifier (CHEETAh)—in essence, a radio frequency amplifier—began as an innovative optoelectronic semiconductor device designed to achieve advanced performance metrics such as a 100 gigahertz (GHz) frequency range far surpassing existing photoconductor and semiconductor switches. Voss and his team sought to demonstrate a semiconductor switch that uses a high-powered laser doped with the base material gallium nitride (GaN) to generate an electron charge cloud while under extreme electric fields. Although the team was ultimately unable to demonstrate results toward this goal by the end of the project, they gained critical knowledge for future optical electronic research and applications.

Semiconductor devices commonly use gallium arsenide (GaAs) as a doping solution to improve laser emissions due to its high refractive index. One unexpected result from the team's earlier experiments using GaAs was a phenomenon called negative differential mobility (NDM). Normally, as increased voltage or field is applied to a semiconductor device, the electrons move faster until they reach velocity saturation, meaning they cannot move any faster because they collide with atoms in the material. However, in this project—still using GaAs—instead of the velocity saturating as voltage is increased, the velocity decreased. The electrons moved slower, and Voss found that he was generating a confined region of electrons that would drift under bias. In normal electron charge clouds, the carriers (electrons) at the front of the cloud shield carriers at the back of the cloud from view and move faster. However, under NDM conditions—when operating in the right regime of laser energy, number of carriers generated, and the applied voltages—the carriers at the back move faster and generate an output voltage pulse that is faster than the input optical pulse. Although the team was able to generate these results using GaAs, they were unable to do so with GaN.

The project's first two go–no-go milestones involved demonstrating the physical principles of the semiconductor and demonstrating the operation at 50 GHz. Voss and his team achieved these two milestones, but the final proof of concept—demonstrating an integrated module before the end of the three-year funding period—was too ambitious. Voss says, "We encountered new regimes of physics that we hadn't anticipated around the negative differential mobility, and we needed to spend more time investigating what that behavior meant. We took an optical pulse and output a shorter electrical pulse, which hadn't been done before and made our aim to reach the high-power levels we initially identified more difficult." Semiconductor device development is an iterative, time-consuming process, a reality that slowed the project's progress. "In hindsight, given the constraints of developing entirely new technology for semiconductors, combined with the constraints to onsite work associated with the COVID-19 pandemic, we were overly optimistic in what we could achieve," says Voss.

The team sees that its work has significant value for future research, which is one of the key benefits of the DR portfolio. "We've learned about the underlying physics of the devices that we're interested in pursuing in the future," he says. "In particular, we learned a lot about operating regimes outside the bounds of where we normally operate. This project will inform how we think about accessing higher frequency modes of operation when building semiconductor devices."



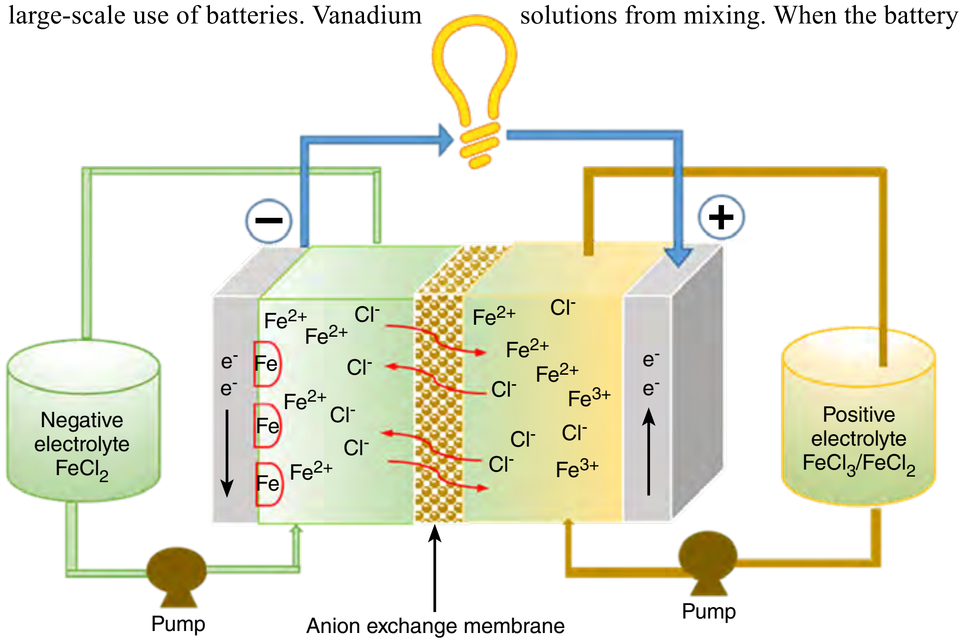
The team tested a semiconductor switch designed to use a high-powered laser doped with gallium nitride (GaN) to generate an electron charge cloud while under extreme electric fields. (Rendering by Lars Voss.)

Powering up Access

Livermore staff scientist Buddhinie Jayathilake doesn't think of an age range when considering her retirement. Instead, she says, "As soon as the entire world has access to low-cost energy, then I'll be ready to retire." Jayathilake's previous work in carbon dioxide (CO_2) conversion and reducing carbon impact has positioned her well to tackle the challenges of her project aimed at finding a cheap and efficient grid-level energy storage solution. A successful outcome could address U.S. national security concerns and drastically increase access to affordable renewable energy around the world.

Realizing cost-effective and efficient renewable energy grid storage has long been a challenge for scientists and engineers. Renewable power sources such as wind or solar are not available all day. According to DOE, viable grid solutions must be able to store excess energy for at least 10 to 12 hours, requiring large-scale use of batteries. Vanadium redox flow batteries are a well-known and reliable battery technology for this purpose. However, at $150 per kilowatt-hour (kWh), vanadium electrolytes are too costly for widespread adoption. Jayathilake is focusing on enhancing iron flow redox battery technology with the use of a device to redistribute lost energy to the system and ensure durability over time. She calls the device an "artificial kidney" because the method in which the device redistributes energy is similar to the way kidney dialysis machines clean and recirculate blood.

Like other flow batteries, iron redox flow batteries use electrochemical reactions of electrolytes (in this case, dissolved iron salts) to store and release energy. Two tanks of electrolyte solutions—one positively and one negatively charged—hold different chemical configurations of iron ions (Fe, Fe^{2+}, and Fe^{3+}). The electrolyte solutions are pumped into a cell stack, wherein a thin membrane prevents the different solutions from mixing. When the battery discharges, iron metal dissolves to the negative solution, releasing electrons (oxidation) and Fe^{2+}, while on the positive electrode the iron ion changes from Fe^{2+} to Fe^{3+} (reduction). To recharge the battery, the process is reversed.



As the redox flow battery discharges, metallic iron (Fe) dissolves into the negative side's electrolyte solution (ferrous chloride) releasing electrons (e-) and iron (II) ions (Fe^{2+}) while iron (III) ions (Fe^{3+}) on the positive side (ferrous chloride at discharged state, ferric chloride at charged state) reduce to Fe^{2+}. Cl^- represents chloride ions. The process is reversed to recharge the battery. (Rendering by Buddhinie Jayathilake.)

Development team for the iron redox flow battery (from left to right): Anna Ivanovskaya, Buddhinie Jayathilake, Hui-Yun Jeong, Marissa Wood, and Alexandra Overland. Not pictured: James Oakdale and Zhen Qi. (Photo by Garry McLeod.)

Iron redox flow batteries have significant advantages over other battery technologies: notably, iron is the most abundant transition metal and significantly cheaper compared to electrolytes in vanadium redox flow batteries. However, traditional iron flow batteries are not durable enough for widespread grid storage use. They tend to lose charging capacity over time as the negatively charged side's reaction differs from that of the positively charged side, resulting in energy loss. To combat this capacity imbalance, Jayathilake's artificial kidney device integrates with the iron redox flow battery system. The device, if successful, will capture the lost energy and store it before electrochemically converting it back to the discharge state and adding it back to the system. Jayathilake says, "This is more sustainable than continuously adding more acids to the systems, which has been the main durability workaround for iron flow batteries to date."

Since the project initiated in April 2022, Jayathilake has successfully tested the artificial kidney device and battery system for quick and intermediate storage tests (1 hour and 5 hours discharging, respectively). Next, her team will test for improved performance over 100 charging cycles, and eventually work toward DOE's storage requirements. If the project is successful and can achieve scale to grid-level solutions, Jayathilake may be able to retire sooner than expected.

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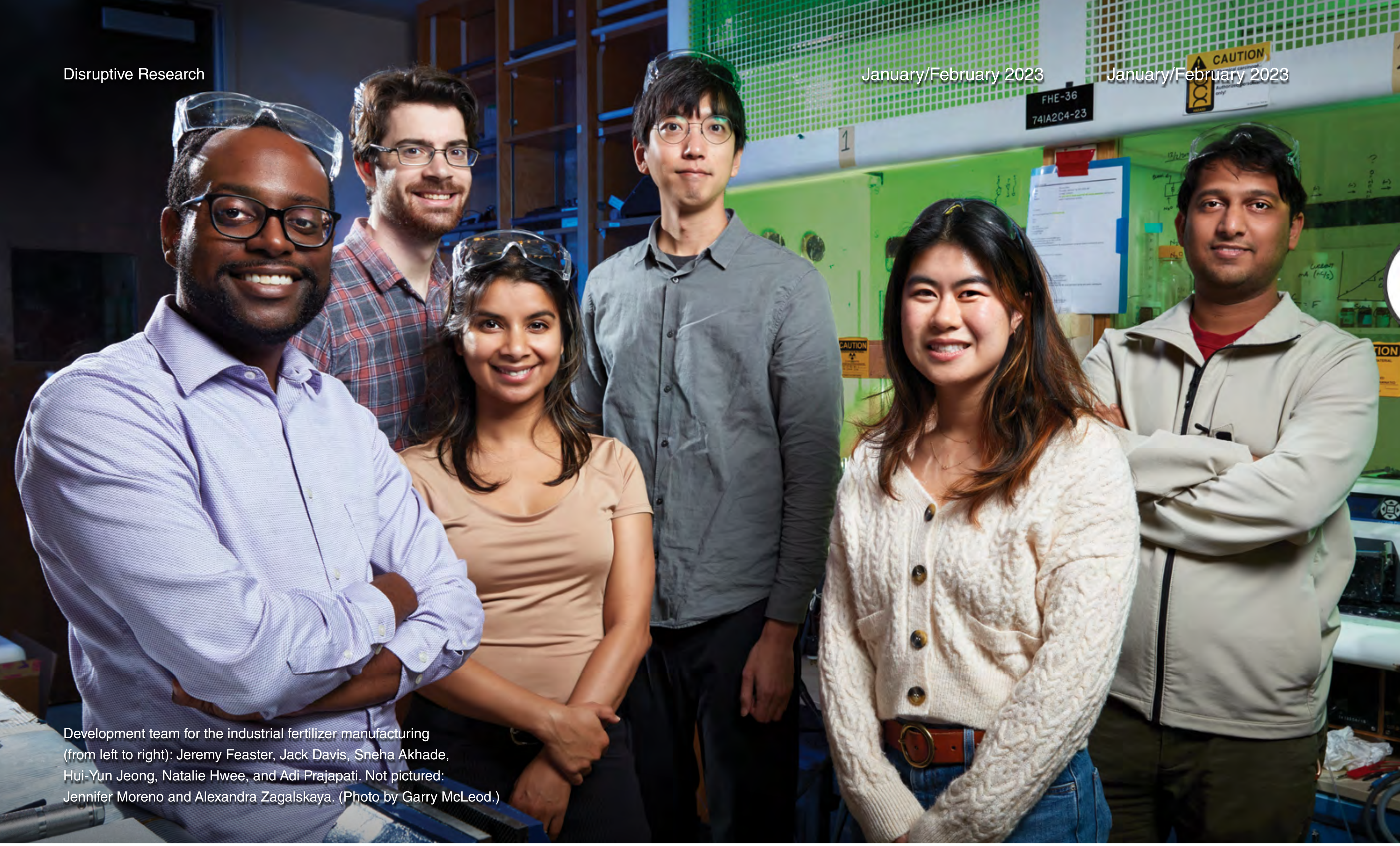


Development team for the industrial fertilizer manufacturing (from left to right): Jeremy Feaster, Jack Davis, Sneha Akhade, Hui-Yun Jeong, Natalie Hwee, and Adi Prajapati. Not pictured: Jennifer Moreno and Alexandra Zagalskaya. (Photo by Garry McLeod.)

Climate Friendly Fertilizer

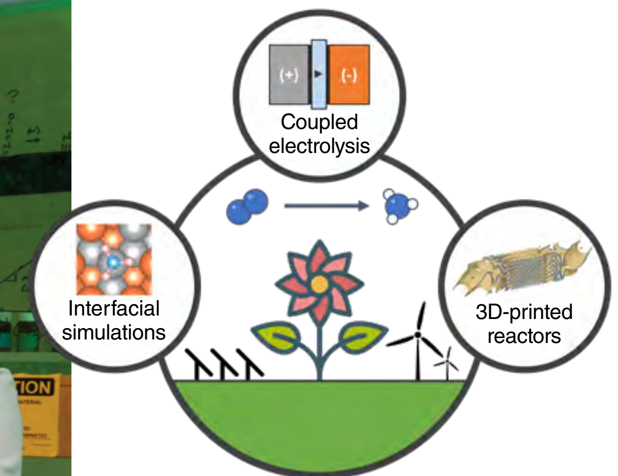
Food insecurity is a daunting challenge made increasingly severe by climate change. Ironically, the process for manufacturing agricultural fertilizers is a major contributor to CO_2 emissions. Industrial fertilizers are manufactured by converting atmospheric nitrogen (N_2) and hydrogen (H_2) into ammonia (NH_3). This process has been instrumental in boosting agricultural production to support the growing global population, but it also emits 1 gigaton of CO_2 annually, all the while consuming 2 percent of the world's energy and 5 percent of the world's natural gas and producing large amounts of greenhouse gas emissions and pollutants.

Lawrence Livermore staff scientist Jeremy Feaster seeks to make the conversion of nitrogen to ammonia greener, more sustainable, and more effective. His novel solution is to convert the air we breathe into ammonia using renewable energy sources and state-of-the-art, additively manufactured electrochemical reactors. If successful, Feaster's technology could initiate a paradigm shift in industrial fertilizer manufacturing and utilization.

Converting nitrogen to ammonia currently involves inducing a thermochemical reaction using a metal catalyst under high temperatures and pressures (between 400 and 500°C and above 10 megapascals, respectively). Nitrogen and hydrogen gases repeatedly pass over four beds of the catalyst and achieve up to 97 percent efficient conversion to ammonia. Although traditional machining methods to fabricate the reactors and catalysts have been effective, efficiency improvements using these methods are limited. Feaster's research leading up to and including the DR project is aimed at accelerating true innovations in electrochemistry.

Feaster's project uses computer assisted design stereolithography to design and fabricate entirely new electrochemical reactors and catalysts in a fraction of the time and for a fraction of the cost of traditional reactors. "With advanced manufacturing, we can design and print systems that only a few years ago were impossible using conventional methods," says Feaster. Traditional reactors require thousands of dollars and weeks to manufacture, and manufacturing new iterations can be a lengthy process. Feaster's research alleviates these limitations, enabling a team to design, print, and test a reactor in a matter of days. If any element does not work, the same process can be used to rapidly develop and manufacture a new iteration for $10 worth of material.

Using the improved process, Feaster and his team are now designing and fabricating electrodes and catalysts in complex structures that offer a much wider range of capabilities in testing new chemical reactions and subsequent outputs. So far, the team's experiments have shown that breaking the extremely strong nitrogen–nitrogen bond is less challenging than activating the nitrogen, which conflicts with past research in this field. Feaster and his team will review these unexpected results and focus their efforts on approaches to activate the nitrogen. The first go–no-go milestone will be tested in April 2023, ideally proving that Feaster's team can achieve a 10-millimolar concentration of activated nitrogen, the same concentration level found in commercial fertilizers. If the trial is successful, the team will advance their focus to converting the activated nitrogen into ammonia.



Livermore researchers are using 3D-printed electrochemical reactors to pursue once-impossible research in industrial fertilizer manufacturing and utilization. (Rendering by Jeremy Feaster.)

Looking ahead, Feaster is optimistic about the potential real-world impact of his research. "We have to think about how we're going to scale this demonstration," he says. "The demonstration is cool, but how do we go from cool to commercial?" Scaling the results will require Feaster and his team to consider size, production, and time requirements to ensure the conversion process can run for weeks and months, not just hours. Feaster has already begun discussions with local farmers about their needs and how the research effort might be tailored to conditions in the field and not just in the laboratory. If the team achieves its project goals, the opportunities for sustainable fertilizer production to support a growing population will expand enormously.

Innovation for the Future

Looking ahead, the DR Program will continue to explore what disruptive research truly represents. The first cycle's projects were almost all successful, owing to the caliber of the research teams' expertise and skills. But, LDRD Program leaders will consider if future projects should push further and embrace even more risk. Livermore's research efforts, scientists, and facilities have all contributed to these successes and demonstrate that the Laboratory can be even more disruptive than imagined. The cultural shift in how scientists picture success is still in its early stages, but Livermore's scientists are increasingly able to be bold and creative. Says Feaster, "Being offered the opportunity to take risks and the grace to fail allows us to shift from a cautious to a more daring approach in which we achieve significant science. We can't solve tomorrow's problems with today's technology. For the technology and solutions needed in the future, we must take correspondingly huge risks."

—Sheridan Hyland

Key Words: Compact High Efficiency Electrically Tunable Amplifier (CHEETAh), computer assisted design, disruptive research (DR) Program, gallium arsenide (GaAs), gallium nitride (GaN), iron redox flow battery, Laboratory Directed Research and Development (LDRD) Program, laser gain medium, metal transpiration cooling, negative differential mobility (NDM), stereolithography, thulium:yttrium-lithium-fluoride (Tm:YLF), vanadium redox flow battery.

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3D Printing Optical-Quality Glass

Livermore development team for tailored glass using direct ink writing (from left to right): Du Nguyen, Jungmin Ha, Timothy Yee, Becca Walton, Oscar Herrera, Rebecca Dylla-Spears, Michael Johnson, Nik Dudukovic, Koroush Sasan. Not pictured: Megan Ellis. (Photo by Garry McLeod.)

2022 R&D 100 WINNER

FROM beads to telescope lenses, glassmaking methods have been honed over millennia to achieve new physical forms with specific optical properties. A glass object is usually created by melting silica powders and hardening the molten mixture in a mold; afterwards, the form can be further modified through subtractive techniques.

Although time-tested, conventional processes limit the range of achievable structures and can introduce structural inconsistencies that corrupt the desired material and optical properties. Instead of subtractively altering glass components after casting, a Livermore research team headed by Rebecca Dylla-Spears has developed glass "inks" to additively manufacture—that is, 3D print—glass components with nearly limitless forms and gradated optical properties.

Breaking the Mold

The team's revolutionary process emerged from a Laboratory Directed Research and Development (LDRD) Program project to bolster optics and laser technology know-how by optimizing the size, weight, and power of integrated components. Until now, glass production methods could not support simultaneous tailoring of complex geometry and refractive index—measurement of the way optical media interact with light. The limited form and performance of traditional optics often requires several individual components be used in combination rather than employing a single, tailor-made component, thereby raising production costs, wasting excess material, and compounding possible error.

The tailored glass using direct ink writing (DIW) method is the first extrusion-based glass fabrication technique to offer the precision of 3D printing alongside the freedom of spatially varying optical properties. DIW is a process of mixing and extruding liquid-phase substances similar to 3D polymer printing (for example, fused deposition modeling). However, far beyond 3D polymer printing, DIW supports a diverse range of materials including ceramics, metals, and now, silica glass. "This technology unlocks a new parameter space ripe for exploration. What we've learned through this work can serve as a springboard for further advanced manufacturing approaches including glass and other multimaterial compositions," says Dylla-Spears.

The process first combines multiple liquid-phase inks into a single glass-forming substance. These specialty inks are composed of solvent (removed post-print) with nanoparticles composed primarily of silicon dioxide and a variety of dopants, for example titanium dioxide or germanium dioxide, that impact the glass's resulting density and refractive index. Carefully controlled flow rates ensure the correct volume of each ink is released to achieve the desired relative concentration at each time step. The separate inks are combined in a micromixer to produce a homogenous substance that is extruded through a nozzle along a programmed path to construct the object. Once printed, the low-density preform, called a green body, undergoes a series of heat treatments to strengthen and condense the build.

The adaptable printing process yields specialty glass structures and optics to work within precise constraints on size, weight, and performance. Structures with variable optical properties address, for instance, the need for intricate, lightweight components in airborne laser–mirror systems. Elsewhere, employing a single flat, refractive index-graded lens in place of an aspheric lens could reduce finishing costs up to 90 percent because fewer unique resources and facilities are needed to produce specialized parts. Maximizing operating parameters while minimizing cost is appealing to aerospace manufacturers and collaborators in the Joint Munitions Technology Development Program between the Department of Defense and Department of Energy. However, the utility of tailored glass goes beyond defense-related purposes. For gemstone purveyor Swarovski, which joined the Livermore team under a cooperative research and development agreement, the technology promises pristine crystal glass with high refractive index and optical dispersion to increase the luster of luxury goods.

The tailored glass by direct ink writing technique preserves fine features while exercising free-form flexibility, as in this 3D-printed helical glass structure.

Convention-Shattering Fabrication

Dylla-Spears's team has already produced an array of complex objects once unthinkable using traditional approaches. The process's free-form flexibility enables fine lattices, solid monoliths, liquid-tight containers, and microfluidic channels, all capable of supporting smooth gradient transitions in color, density, and refractive index. While the components are manufacturing marvels in their own right, Dylla-Spears explains, "I expect the technology will complement conventional optics fabrication processes. Customers are likely most interested in custom containers, gradient optics, and lightweight mirror blanks." The process's high customizability will allow manufacturers to rapidly prototype and improve glass-based designs.

Developing the technology was all but straightforward. Dylla-Spears says that preventing cracks posed a significant challenge when printing at large scales and with composition gradients. "Initially, we sought to optimize handling and heat treatment protocols around a proven ink formulation," she says. "Recently, however, we shifted focus to making the ink formulation itself more robust to cracking, which has allowed us to increase the optical area by almost 10 times."

After establishing feasibility of 3D-printed glass, Livermore materials engineer Du Nguyen focused on multimaterial patterning and extrusion consistency. Achieving an accurate multimaterial composition profile proved particularly challenging because ink deposition rates must continually fluctuate to yield gradient properties. "Effects such as residence time in the nozzle and capacitance throughout the system impact ink deposition rate," says Nguyen. The team attempted to match ink rheology and to minimize air bubbles but found that minute inconsistencies are inevitable. Nguyen explains, "We countered these effects by using a microfluidic circuit analogy to program deposition to actively compensate for encountered inconsistencies."

Staff scientist Timothy Yee, who worked alongside Nguyen, also concentrated on post-print processes. "Fine tuning the heat treatment process was vital to converting printed parts into fully dense, transparent glass," says Yee. The heating process required careful design to ensure that all solvent and organic contaminants are removed and to minimize cracking and warping during sintering. Once cooled, mechanical engineer Megan Ellis characterized the products using dimensional analysis to validate printing accuracy and understand structures' reactions to applied forces. "Due to factors such as interstitial spacing and residual stresses, 3D-printed parts sometimes exhibit more structural flaws than a comparable piece of the bulk material," says Ellis. "We iteratively improved aspects such as formulation, printing orientation, and consolidation to ensure higher quality products."

Nguyen maintains that the award-winning process could only have been achieved through the project's multidisciplinary team effort. He says, "Glass manufacturing is an ancient process, a part of human history, and continuing that history by developing new ways of working with the material is incredibly exciting."

—Elliot Jaffe

Key Words: additive manufacturing, direct ink writing (DIW), optics, R&D 100 Award, refractive index, tailored glass.

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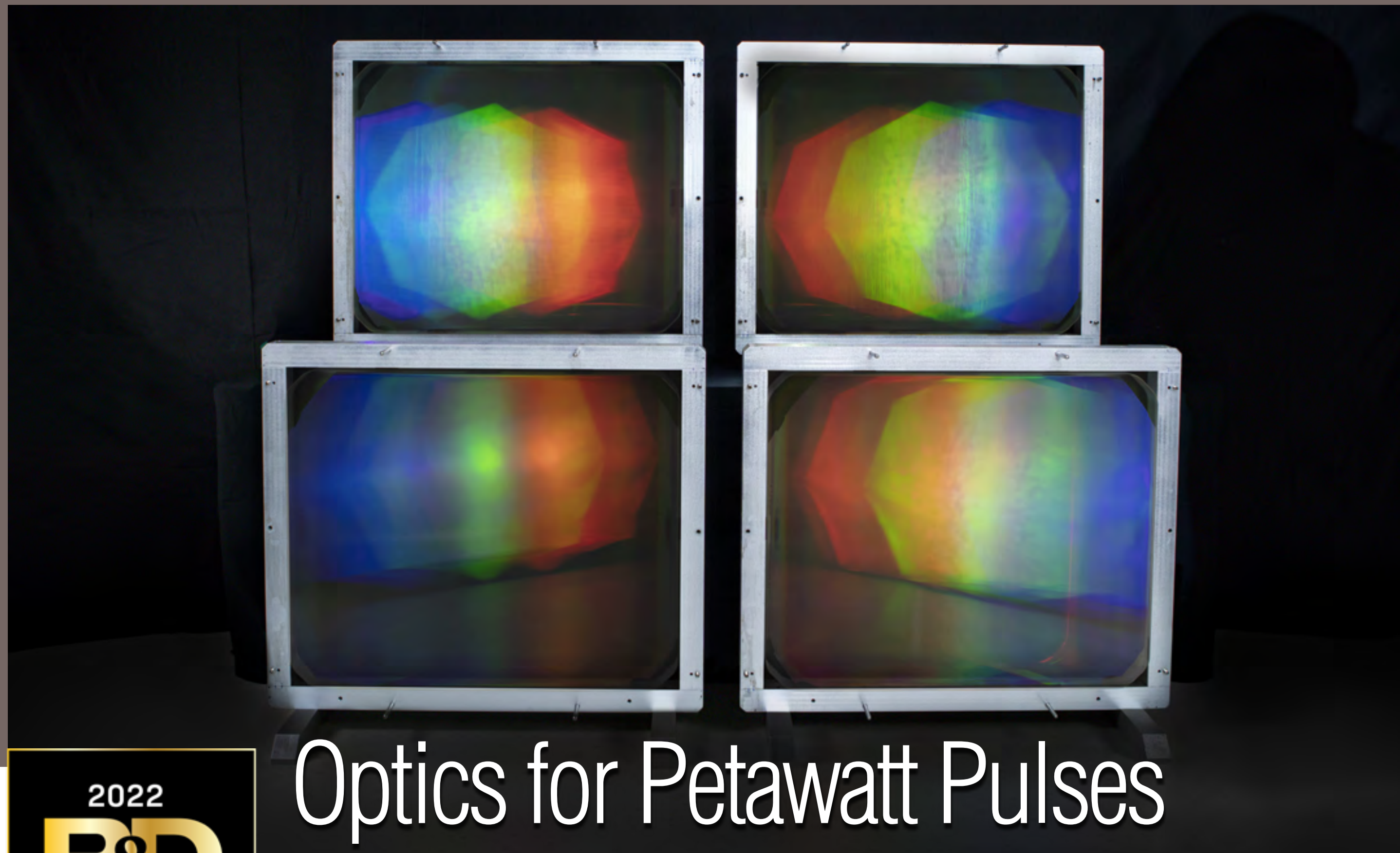

Meter-sized high-energy, low-dispersion (HELD) gratings will be installed in the ELI Beamlines L4-ATON laser system.

Optics for Petawatt Pulses

As the home of the world's largest and most energetic laser, Lawrence Livermore regularly stands at the forefront of high-energy-density physics research. The Laboratory's laser systems create extreme experimental conditions by exploiting a simple relationship: power is defined as energy transfer over time. By constraining a large burst of energy to a nearly instantaneous time frame, power grows enormously, allowing researchers to briefly mimic the intense environments of solar interiors and black hole horizons.

Through the Nobel Prize–winning method known as chirped-pulse amplification (CPA), scientists can spectrally and temporally stretch a short initial laser pulse, energize it, and finally compress it once again to produce a concentrated, high-energy blast. CPA warps and redirects light using a series of diffraction gratings—multilayer reflective panels composed of a base substrate and stacked films of dielectric material.

Such immense power cannot be generated nor withstood by just any ordinary gratings. Livermore senior laser scientist Hoang Nguyen has spent years researching technological solutions to identify laboratory equipment that can endure repeatable laser-based experiments involving petawatt (10^{15} watts) power levels. "Laser systems are breaking into the petawatt regime and allowing us to consider previously untenable experiments. While this is exciting news for scientists hoping to learn more about exotic physics, designing and manufacturing the right hardware to cope with these extreme energy levels is an incredible challenge," says Nguyen. Joined by industry partners, Nguyen's team at Livermore devised high-energy, low-dispersion (HELD) gratings made solely of multilayered dielectric materials that can withstand higher input laser energies than ever before.

Powering the Petawatt Era

According to Nguyen, HELD gratings can tolerate up to 3.4 times the incident energy of previous gratings to work effectively in emerging ultrafast laser systems, namely, the ELI Beamlines L4-ATON laser under construction in Prague, Czechia. Using HELD gratings, the laser will be able to fire off a 1.5-kilojoule laser beam in just 150 femtoseconds (10^{-15} seconds) to generate up to 10 petawatts of peak power. Performing CPA on this ultrahigh intensity setup will enable researchers to observe and better understand exotic astrophysical and quantum phenomena, namely gamma-ray flashes, electron–positron pair generation, radiation–friction force, relativistic flying mirrors, Unruh physics, and vacuum birefringence. Scientific insights could aid understanding of cosmic acceleration and quantum gravity. In the long term, incorporating plasma lenses could yield lasers with intensities approaching the Schwinger limit, above which electromagnetic fields are thought to become nonlinear.

Through technological innovation, Nguyen's team is driving the next generation of physics research, which can only be conducted with the world's most sophisticated lasers. Attempting to understand physical behavior at mindboggling scales of time and energy is a matter of conjecture unless researchers are provided with the right equipment. High-energy experiments such as those performed at Livermore's National Ignition Facility (NIF) rapidly degrade even the sturdiest hardware; NIF's components are regularly swapped out due to the sheer intensity of operation. "HELD grating technology is the culmination of significant investment from the Laboratory and our partners," says Nguyen. "The gratings we have fabricated will support laser systems at an unprecedented level of peak power. Seeing this project through to the end required a massive amount of infrastructure, custom-built equipment, and complex workflows."

Livermore development team for HELD gratings (from left to right): Sean Tardif, James Nissen, Hoang Nguyen, Candis Jackson, and Brad Hickman.

Scrupulous at Scale

Investment in each stage of the innovation helped Nguyen and his team navigate a host of challenges bridging laser theory, engineering, and logistics. At nearly one square meter, HELD gratings dwarf most optical components. The team devoted significant effort to scaling up methods and designs to such large proportions while maintaining submicrometer manufacturing precision. For example, they needed to carefully control the lithographic exposure process for the entire surface to exhibit the greatest possible spectral uniformity.

The team faced further challenges when carving out the gratings' surface profile, which is responsible for morphing the spectral and temporal characteristics of incident light to perform CPA. Each millimeter of the final grating surface contains more than 1,000 carved-out valleys of varied depth and spacing tailored to the specifications of each laser system. "Our meticulous process maintained ion-beam etching uniformity over an 80-centimeter aperture," says Nguyen, because the etching technique is not often applied to the grand scale of HELD gratings. "Beyond fabricating components with the desired specifications, we had to figure out the logistics of safely handling 136-kilogram optics throughout each step in the first place."

Nguyen and his team ultimately produced the gratings through a Strategic Partnership Project with ELI Beamlines and a collaboration with the Optical Coating Group at Spectra Physics. "The partnership with ELI Beamlines and Spectra Physics was essential to bringing the gratings to full scale," he says. "The HELD technology emerged from four years of research and development rooted in collaboration and substantial support from Livermore's NIF and Photon Science Principal Directorate." With imminent integration into the ELI Beamlines project, Livermore's HELD gratings will bring the next echelon of physics research into view.

—Elliot Jaffe

Key Words: high-energy, low-dispersion (HELD) grating; laser; multilayer dielectric; National Ignition Facility (NIF); optics; petawatt; R&D 100 Award.

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Powering Next-Generation Energy Storage Devices

Livermore development team for Energy Inks (from left to right): Marcus Worsley and Swetha Chandrasekaran. (Photo by Garry McLeod.)

2022 R&D 100 WINNER

WORLDWIDE demand for electronics is surging. So, too, is reliance on the energy storage components that power them. Shrinking device sizes coupled with the need for longer charge life and better performance have spurred research efforts into battery designs that not only meet escalating benchmarks but do so economically and with fewer harmful byproducts.

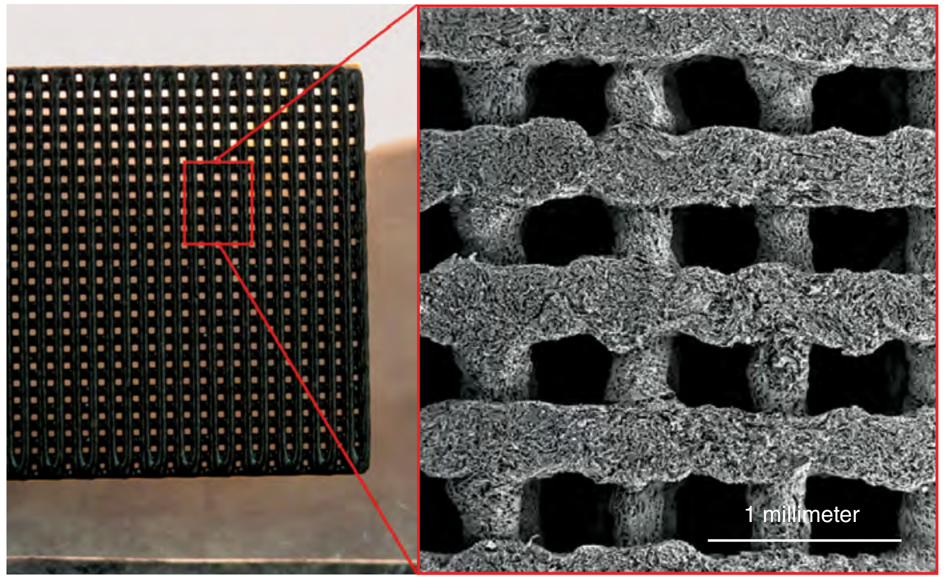
To address this growing challenge, a Livermore-led effort drew upon the Laboratory's additive manufacturing expertise to enable effective 3D printing of functional energy storage devices. Specially formulated feedstock materials, Energy Inks, will equip manufacturers with the tools to rapidly explore new designs of batteries and supercapacitors in addition to devices used in catalysis, filtration, and remote sensing.

Charging Ahead

Energy Inks rely on the increasingly popular process of direct ink writing (DIW), which enables extrusion and deposition of materials including metal, glass, and ceramics to build objects in unparalleled, 3D forms. Applying DIW technology to energy storage devices in particular will allow researchers and manufacturers to optimize components for operation within specific size, performance, efficiency, and cost constraints. "At Livermore, we constantly develop advanced materials with functional and improved properties," says staff scientist Swetha Chandrasekaran, who headed the award-winning Energy Inks project. "Many of these materials are reserved for the Laboratory's mission space, but our project has global applications."

While 3D printing of solid-state electrode architectures has been achieved, Energy Inks introduces direct printing of fully operational components. Printing functional devices such as batteries with DIW requires a carefully designed ink formulation that retains the desired device characteristics both during extrusion and after hardening. Chandrasekaran explains, "Controlling the composition and rheological behavior of the feedstock inks is crucial to forming self-supporting filaments that maintain their shape as they span over previously deposited layers. To fabricate parts from a variety of materials, each ink must be tailored to deliver the optimal combination of rheological properties, such as viscoelastic response and shear thinning." The result is a method that supports customized properties and lowers manufacturing cost.

Support such as that from the Department of Energy's Technology Commercialization Fund (TCF) enabled the team to develop materials that could be made available for academic research institutions and commercial users. "I'm especially thankful to business development experts in the Laboratory's Innovation and Partnerships Office—Genaro Memphin and Annemarie Meike (now retired)—for assisting in the TCF collaboration with industry partner MilliporeSigma," says Chandrasekaran.



A component printed with Energy Inks graphene oxide product (left) retains the material's characteristic porous quality (right) and related functionality.

MilliporeSigma now offers three Energy Inks in the marketplace. The first, graphene oxide (GO), is used as an electrode material in lithium-ion batteries, supercapacitors, and electrocatalytic devices. Based on GO nanosheets, the ink promises fast charge rates, increased cycle life, and improved gravimetric capacitance for next-generation energy storage devices. In 2020, Chandrasekaran's team collaborated with researchers from the University of California at Santa Cruz to build a graphene aerogel electrode. The component overcame traditional limitations of supercapacitors to achieve the highest areal storage capacitance to date, reaffirming the potential of extrusion-based architectures.

Enabling High Performance

The remaining two Energy Inks are composed of ceramic microparticles to withstand harsh conditions. The team's yttria-based zirconia (YSZ) ink is designed to operate within chemically corrosive, low-pH environments. YSZ's tunable porosity and high surface area make the ink best suited for filtration, catalysis, and thermal insulation. The ink also presents great utility as a retrofitting material in existing energy storage, conversion, separation, and sensing devices. The mechanically robust B_4C ink, on the other hand, exhibits a unique combination of lightweight and ultrahigh temperature resistance, making it ideal for high-wear components and heat exchangers in settings such as nuclear reactors and lightweight body armor. While robust once printed, both liquid inks exhibit high viscosity and stable dispersion to enable a smooth printing process.

Staff scientist Alyssa Troksa focused on optimizing YSZ ink for use in membranes and filters as well as characterizing its long-term stability. Working alongside MilliporeSigma required regular testing and data sharing of rheological behavior and extrudability to ensure consistent compositional quality. Troksa says the team needed to find a way for ceramic nanoparticles to remain dispersed and suspended over long periods of time. "We tuned the relative concentrations of nanoparticles and polymer binders and additionally adjusted storage conditions and mixing procedures until we found a formulation best suited for printing and performance," she says. Each ink was analyzed to ensure a shelf-life of at least 10 months for inclusion in the MilliporeSigma product catalogue.

Materials scientist James Cahill, who worked on the B_4C ink design, describes intricacies of the development process. "The main challenge was ensuring sufficiently high solids loading of particles to enable sintering to near-full density," he says. "However, because solids loading affects viscosity, and therefore printability, the process is full of trade-offs." He says the team achieved between 50 and 60 percent solids loading by volume, which optimized the sintering process while maintaining printability.

With applications as diverse as consumer electronics, transportation, and medical devices, printable energy materials will empower researchers and industries to incorporate novel approaches when conceiving new energy technologies. Energy Inks' customizability and low relative cost to traditional manufacturing techniques present innovators with a powerful tool to help facilitate a broad transition to clean, efficient, and effective energy storage components. "Seeing Energy Inks translated from the benchtop to a commercially available product was extremely fulfilling as a scientist," says Troksa. "We're helping shape and drive growth of the high-performance energy device field. I'm excited to see what people will create with this technology."

— Elliot Jaffe

Key Words: additive manufacturing, battery, ceramic, direct ink writing (DIW), energy storage device, Energy Inks, functional device, MilliporeSigma, R&D 100 Award, supercapacitor.

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S&TR January/February 2023

TRACING A DECADE OF GROWTH

ACCOLADES such as R&D 100 awards rarely represent a technology's climax, but rather its beginning. DNATrax, which garnered a 2013 R&D 100 Award for Livermore, touted aerosol particle traceability with unparalleled accuracy. (See *S&TR*, October 2013, pp. 4–5.) The technology's subsequent path to commercialization and applications in both agriculture and indoor air quality epitomizes the potential of Laboratory inventions to transcend early scope and function. "I'm a physical chemist and an aerosol expert, not a biologist," says inventor and former Lawrence Livermore scientist George Farquar. "This work might not have come to fruition without an out-of-the-box approach to the challenge of airborne particle tracing."

The technology's novelty is in its DNA—literally. Short for DNA-Tagged Reagents for Aerosol eXperiments, DNATrax utilizes sugar-based microparticles no larger than 10 micrometers in diameter to safely mimic the size and shape of airborne contaminants. Researchers laced these microparticles with a short sequence of non-coding, synthetic DNA (roughly 100 base pairs) that functions like a barcode, only with nucleotide bases in place of digits. The microparticles, manufactured with Food and Drug Administration–approved ingredients, contain a unique identifier allowing researchers to distinguish them from other airborne matter once dispersed. After releasing DNATrax particles, collecting air samples and using a standard polymerase chain reaction technique to amplify DNA nametags to testable volumes allows experts to map airflow patterns inside a building by tracing particles' paths from start to end.

Breaking Out

The first big break for DNATrax came during a biodefense conference. Farquar's well-rehearsed, 30-second elevator pitch convinced a prospective funder of the technology's potential. With funding from the Defense Threat Reduction Agency, Farquar and his team advanced the technology from concept to product through significant research and development efforts. "Our human resources ultimately made this technology possible," says Farquar. "Our researchers, program managers, and administrative team moved the project through testing and a mountain of paperwork, even while facing logistic complications from Hurricane Sandy. I cannot say enough good things about our team."

No longer confined to the walls of Livermore's laboratories, DNATrax was soon deployed in the hallways of the Pentagon and on New York City subway platforms to predict the effects of a hypothetical bioterrorism event. Research teams analyzed large, interconnected structures to pinpoint vulnerable entry locations and stagnant air regions where harmful substances could concentrate and pose significant hazards.

In coordination with the Pentagon Force Protection Agency, researchers released DNATrax microparticles—multiple types of particles with unique DNA barcodes—to reveal air circulation or stagnation resulting from the Pentagon's heating, ventilation, and air conditioning systems.

Originally conceived as a security and defense solution, the researchers—and investors—quickly realized the invention's broader applicability. DNATrax presented a risk-free way to evaluate private, public, and government properties for the dangers of many aerosolized substances, including pathogens, combustive products of wood-burning stoves, tobacco, and potent chemicals including formaldehyde and asbestos. "After the 2013 R&D 100 Award, we received loads of press, including a story in the *New York Times*, and interest in the technology took off from there," says Farquar.

Seeing the growing popularity of DNATrax, Farquar eventually left Lawrence Livermore to establish a company based on the innovation and serve as Chief Technology Officer. He says, "The Laboratory prepared me to be a better entrepreneur by teaching me how to seek funding and approach problems in unique ways. After learning the ins-and-outs of government research operations, I'm unfazed by complex processes concerning regulation, certification, and intellectual property for a product."

Agricultural Use Reaches Fruition

The next step, commercialization, represented a major turning point for the technology. In 2015, the company reincorporated under the name SafeTraces and pivoted to a new mission: ensuring product quality and integrity in the agricultural industry. Ulrike Hodges, Chief Operating Officer and founding member of SafeTraces, understood that global agricultural systems face issues of product adulteration, labor exploitation, and environmental destruction. SafeTraces' particle tracing technology offered a glimpse into the weakest links of food supply chains by applying innocuous amounts of DNA-tagged particles (made primarily of harmless, ingestible sugar) at a harvest or production site. The ability to trace individual grocery items to their source exposed whether the product had been contaminated, swapped, or diluted; whether it was associated with exploitative labor practices; and whether its region of origin was flouting environmental regulations.

Chief Executive Officer Erik Malmstrom joined SafeTraces in late 2018 as the company focused on food production and distribution challenges. He says, "We saw a huge opportunity for product traceability to address vulnerabilities and inefficiencies in preventing, detecting, and responding to pathogens entering food chains as well as issues with counterfeiting and adulteration. We could also meet consumer demand to know how and where food is produced, spotlighting food chains with a history of environmental and labor abuses, such as palm oil. SafeTraces countered earlier, flawed approaches with safe, edible, invisible DNA barcodes applied directly and cost-effectively on food products."

The SafeTraces team presents air quality-related features of the technology at the 2022 International Facilities Management Association conference in Nashville, Tennessee.

Change Is in the Air

Agriculture remained SafeTraces' priority until the COVID-19 pandemic emerged and shelter-in-place orders prevented SafeTraces technicians from performing commercial tracer applications. The company examined the emerging "new normal." The specter of infection spread by airborne particles demanded individuals and businesses avoid crowded indoor spaces, maintain physical separation, and provide contact tracing. Interest grew in indoor air circulation improvements and identifying problematic building layouts and inefficient heating, ventilation, and air conditioning equipment.

Recognizing a sudden, pronounced need for effective indoor air quality mapping, SafeTraces revisited the proprietary technology's original application and elected to focus exclusively on air quality assessment. Malmstrom champions the company's unique, tangible solutions. "I see a great deal of pure software and analytics solutions in the marketplace, but fewer companies are developing applied diagnostics that generate high-quality data to derisk the vulnerability of software- and data-based solutions," he says. "We're a mission-focused company in that we provide these services not just to the best-funded customers, but the spaces that need improved air quality most such as mass transit systems, public schools, prisons, and low-income housing developments. We seek to partner with disproportionately underfunded groups—not just Fortune 100 companies—to make the greatest difference."

In November 2022, SafeTraces received a Phase II Small Business Technology Transfer contract from AFWERX to monitor air quality at U.S. Air Force healthcare sites. Farquar, who has since founded another substance detection company, notes, "Inventing a technology that continues to grow in impact a decade later is nothing short of amazing." Such success signals this year's awardees that scalability and social benefit are within reach.

— Elliot Jaffe

Key Words: aerosol, airflow, air quality, contact tracing, COVID-19, DNATrax, microparticle, R&D 100 Award, SafeTraces.

Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven- or eight-digit number in the search box at the U.S. Patent and Trademark Office's website (uspto.gov).

Patents

Magnetic Nanostructures and Composites for Millimeter Wave Absorption
Jinkyu Han, Thomas Han
U.S. Patent 11,404,793 B2
August 2, 2022

Shape Memory Embolectomy Devices and Systems
Jason Szafron, Duncan Maitland, Ward Small, IV, Patrick Buckley, Andrea D. Muschenborn
U.S. Patent 11,406,401 B2
August 9, 2022

Liquid-Free Polymeric Reinforcement of Nanoscale Assemblies
Javier N. Lepro Chavez, Chantel M. Aracne-Ruddle, Salmaan H. Baxamusa, Michael Stadermann
U.S. Patent 11,408,074 B2
August 9, 2022

SI-Based CTE-Matched Substrate for Laser Diode Packaging
Susant Patra, Robert J. Deri, John W. Elmer
U.S. Patent 11,411,370 B2
August 9, 2022

Flow-Through Electrode Capacitive Deionization Cell
Patrick G. Campbell, Jennifer M. Knipe, Michael Stadermann
U.S. Patent 11,411,663 B2
August 9, 2022

Monolithic Rare Earth Oxide Aerogels
Marcus A. Worsley, Alexander E. Gash, Robert A. Reibold
U.S. Patent 11,414,598 B2
August 16, 2022

Indirect Conversion Nuclear Battery Using Transparent Scintillator Material
Joshua Jarrell, Nerine Cherepy, John Winter Murphy, Rebecca J. Nikolic, Erik Lars Swanberg, Jr.
U.S. Patent 11,415,713 B2
August 16, 2022

Optimization Control Technology for Building Energy Conservation
Yining Qin
U.S. Patent 11,416,739 B2
August 16, 2022

System and Method for Control of Compression in Internal Combustion Engine via Compression Ratio and Elastic Piston
Daniel L. Flowers
U.S. Patent 11,428,174 B2
August 30, 2022

Time-Gated Fast Neutron Transmission Radiography System and Method
Andrea Schmidt, Maurice B. Aufderheide, David Neal Fittinghoff, James M. Hall, Yuri Podpaly
U.S. Patent 11,428,831 B2
August 30, 2022

Awards

A multi-laboratory **Burning Plasma Team** that included numerous Livermore researchers received the **John Dawson Award for Excellence in Plasma Physics Research** for cutting-edge experimentation performed at the National Ignition Facility (NIF). Presented by the **American Physical Society**, the award recognizes the first laboratory demonstration of a burning deuterium-tritium plasma where alpha heating dominates the plasma energetics. The team's work in inertial fusion, detailed in the January 26 issue of *Nature Physics*, signified a key milestone in attaining the 1.3 megajoule yield at NIF in August 2021 and the promise of progress in the pursuit of self-sustaining fusion energy.

Laboratory plasma scientist **Alison Ruth Christopherson** earned the **American Physical Society's** (APS) **Marshall N. Rosenbluth Outstanding Doctoral Thesis Award** for her work describing theoretical foundations of fusion alpha heating and metrics applied to thermonuclear ignition in inertially confined plasmas. The award, named for a famed fusion plasma theorist, recognizes original thesis work of outstanding scientific quality and achievement in plasma physics and includes an invitation to speak at the annual meeting of the APS Division of Plasma Physics. Livermore's **Omar Hurricane** co-nominated Christopherson for the award citing her important efforts to confirm theory with both experiments and simulations.

Abstract

Big Risks and Bold Science

The Disruptive Research (DR) Program, launched in 2019 as a new component of Lawrence Livermore's Laboratory Directed Research and Development Program, supports research and development activities that are unconventional, innovative, and at the forefront of their fields. In DR projects, Livermore researchers are encouraged to embrace high levels of technical risk to yield transformative scientific advances. Even if the stated goal of a project is not met, the DR Program recognizes the contribution of higher risk experiments to producing order-of-magnitude improvements, opening new program spaces, or creating positive impacts in Laboratory initiatives. As the first cycle of selected DR projects reaches completion and the second approaches go–no-go milestones, program researchers reflect on discoveries made, lessons learned, and next steps in disruptive research designed to advance food production, energy storage, laser science, and hypersonic flight.

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Double Asteroid Redirection Test (DART)

Lawrence Livermore contributed multiphysics simulations supporting NASA's successful experiment to divert an asteroid.

Also in an upcoming issue…

- *Livermore's capabilities in flight dynamics simulations define the effects of warhead design prior to flight testing.*
- *Sidney Fernbach Postdoctoral Fellows contribute computational science research and attract new talent for the future.*
- *Laboratory additive manufacturing expertise yields a training resource for bomb-sniffing dogs.*

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