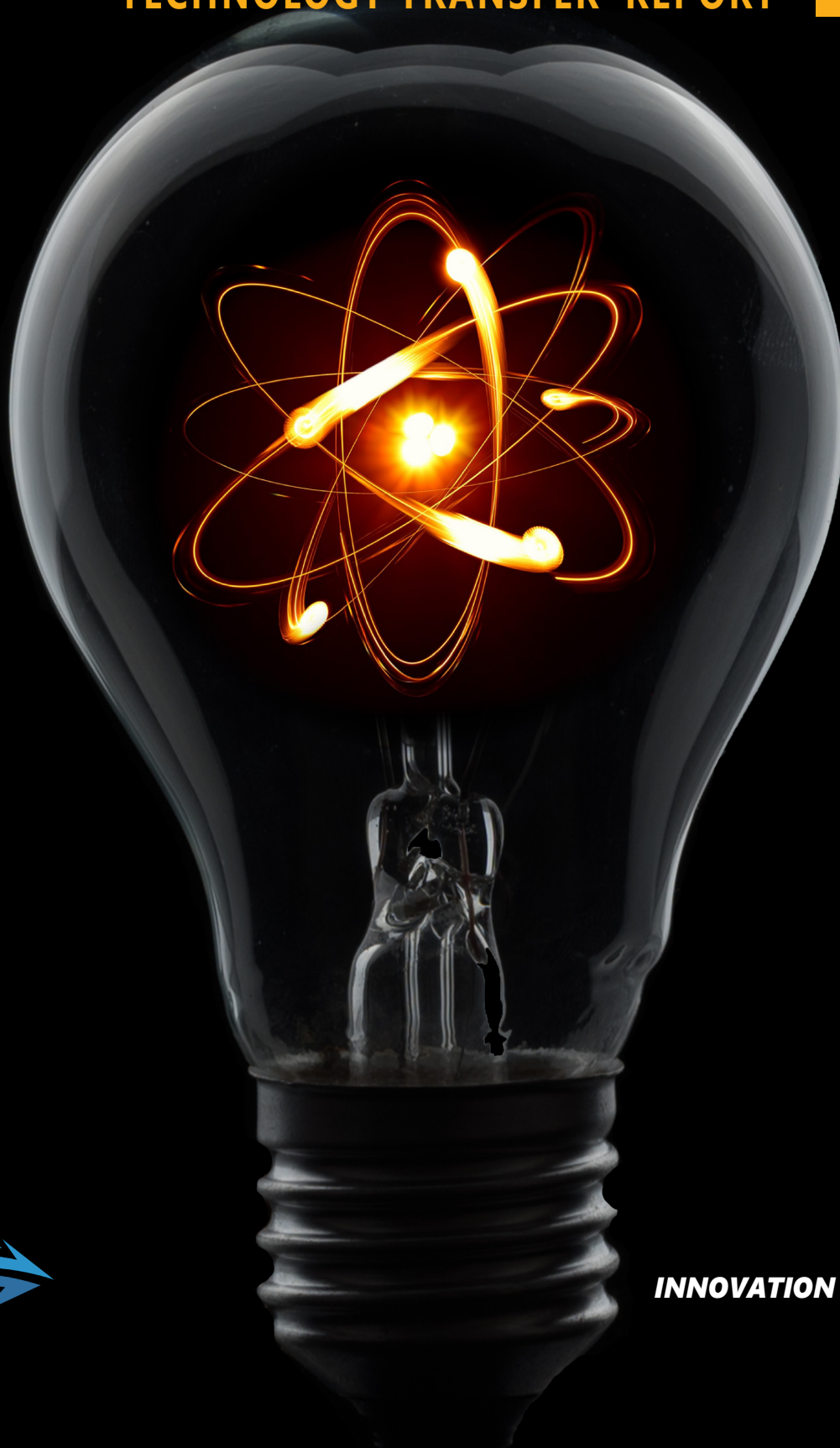


FY23

**Lawrence Livermore
National Laboratory**

TECHNOLOGY TRANSFER REPORT



INNOVATION & PARTNERSHIPS OFFICE



INNOVATION IN ACTION



LAWRENCE LIVERMORE
NATIONAL LABORATORY
INNOVATION AND
PARTNERSHIPS OFFICE

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*written contributions provided by Sheridan Hyland,
Elliot Jaffe, Lilly Ackerman, and Suzanne Storar*

Photo

Home of IPO - Office Building (Bldg. 642) & Conference Annex (Bldg. 643), part of LVOC, Livermore Valley Open Campus (Garry McLeod).

LLNL is managed by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration, under contract DE-AC52-07NA27344.

LAWRENCE LIVERMORE NATIONAL LABORATORY

IPO'S NEW DIRECTION



The Innovation and Partnerships Office (IPO) has seen a number of changes in FY23 – many of which you can read about in this annual report. We have reimagined our annual report to focus more clearly on IPO activities so that we may share our impact more effectively with the LLNL community. And we have observed a greater interest in the scientific discoveries that LLNL scientists make, and IPO is managing an increasing number of requests for licensing and partnerships. One of our biggest initiatives this fiscal year is the procurement and deployment of a new intellectual property (IP) asset management platform. Scheduled to be operational next year, this platform will revolutionize the way that we report inventions, manage agreements, and track industry interactions. Look out for news of its release later in FY24!

Elsie Quait-Randall

ELSIE QUAITE-RANDALL
Deputy Director, IPO



IPO is one of the key contributors to the innovation ecosystem at LLNL, facilitating external partnerships that enable the technologies developed at LLNL to contribute to U.S. economic and national security via technology transfer. Achieving fusion at the National Ignition Facility (NIF)—first in 2022 and again in 2023—in combination with an increased national focus on clean energy transition has increased IPO industry engagement and technology deployments. Innovations deployed from LLNL in areas such as advanced manufacturing, life sciences, electro-optics, and materials science are making a powerful economic and national security impact, leading to significant public investment and job creation. The enclosed annual report reflects the incredible contributions in FY23 of LLNL staff, scientists, engineers, and senior leadership towards the technology transfer mission. We invite you to engage with IPO if you are interested in leveraging LLNL's world-class innovation ecosystem and capabilities.

Matt Garrett

MATT GARRETT
Director, IPO



INNOVATION & PARTNERSHIPS OFFICE **AT A GLANCE**

FY2023

The Innovation and Partnerships Office (IPO) at LLNL is charged with ensuring that discoveries made at the Lab through mission-driven scientific research have the maximum impact on U.S. industrial competitiveness and the American public. IPO manages this through its three "P's" for technology transfer: Protection, Partnerships and Programs.

PROTECTION – Initiating steps to impact. IPO reviews and assesses the potential commercial impact of intellectual assets reported to their office. This assessment involves technical diligence, patentability, and market analysis. If the intellectual asset shows promise, IPO will invest Lab resources to formally protect the intellectual asset through patent protection or copyright registration.

PARTNERSHIPS – Developing LLNL discoveries for deployment. IPO understands that the Lab's intellectual assets are often very early-stage and that additional work needs to be performed in order for our discoveries to be deployed in the commercial world. IPO works with LLNL innovators to develop technology roadmaps that can help them identify potential industry partners, and then reach out to the most promising partners.

PROGRAMS – Enabling the entrepreneurial ecosystem. IPO delivers entrepreneurial training for the LLNL community on a regular basis and interacts with other members of the DOE/NNSA complex on several entrepreneurial activities. IPO is also a key player in the development and management of a variety of technology deployment programs designed to move early stage technologies to the next level.

Photo top

IPO Team group photo (Garry McLeod).

Photo bottom

IPO Team discussing IPO goals (Garry McLeod).



OUR VISION

IPO engages and facilitates partnerships with internal & external customers to deliver mission-driven solutions. In addition to strategically protecting LLNL innovations, the team fosters equitable engagements that enhance economic security and stimulate U.S. competitiveness.

OUR MISSION

Our purpose is to facilitate access to Livermore's unique innovation ecosystem for the private sector, creating value for the U.S. by proactively accelerating and transferring LLNL innovative science and technology to industrial partners.

OUR VALUES

IDEAS
Shared

IPO shapes the Lab's innovation with market-based assessment and consistent implementation of new business models for technology transfer and commercialization.

IMPACT
Maximized

IPO fosters collaboration leading to positive impact on the U.S. economy through innovative contractual solutions.

INTEGRITY
Focused

To ensure transparency and honesty, each IPO Team member strives to be the "go-to" person in matters related to innovation and partnerships.

ZEAL
Enduring

IPO helps create global impact from our bold and innovative science and technology. Our societal impact raises enthusiasm for and commitment to the Lab's missions.

INCLUSIVENESS
Matters

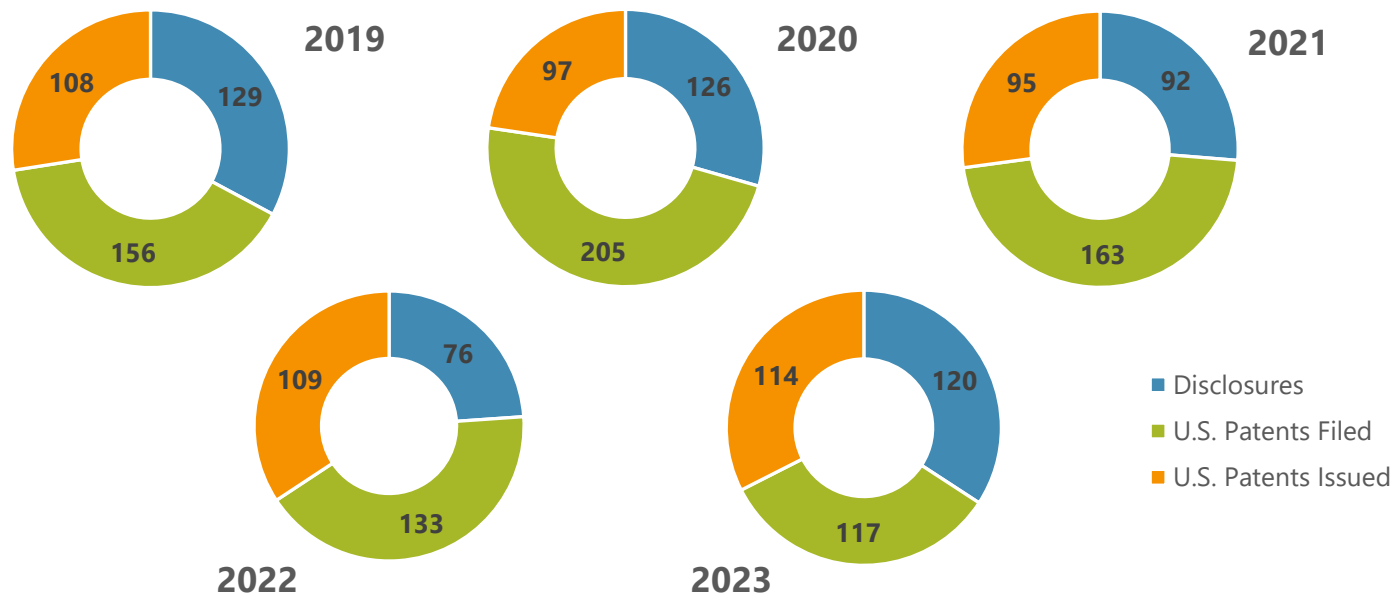
IPO excels at sharing information and communicating while allowing team members to bring their unique contributions.



KEY FIGURES METRICS

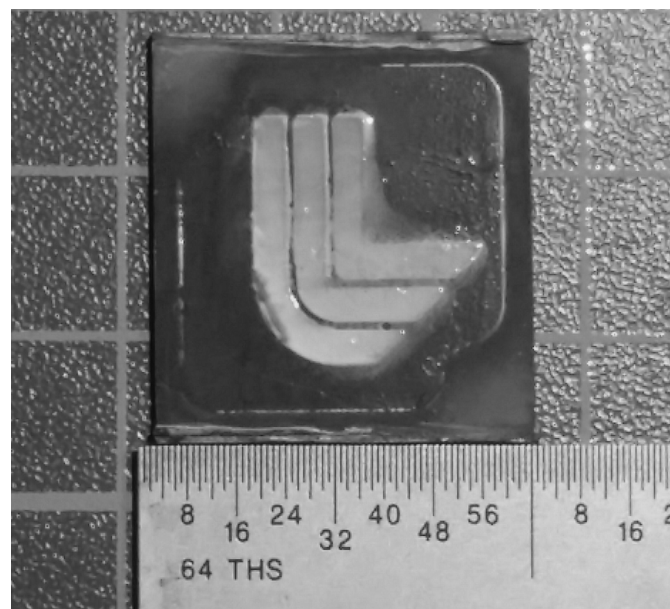
INTELLECTUAL PROPERTY

LLNL-based inventions are protected by more than 1,000 issued patents and patent applications, including provisional patents, from 2019 to 2023.

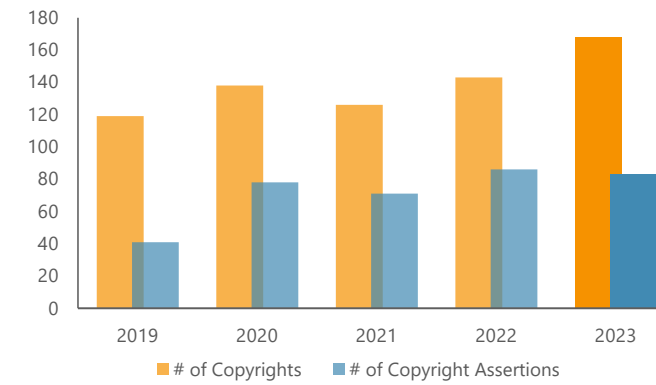


These are some of the ways we measure the successful technology transfer from LLNL to commercial partners.

Photo
This proof-of-concept logo was 3D printed using light-directed electrophoretic deposition (LLNL).

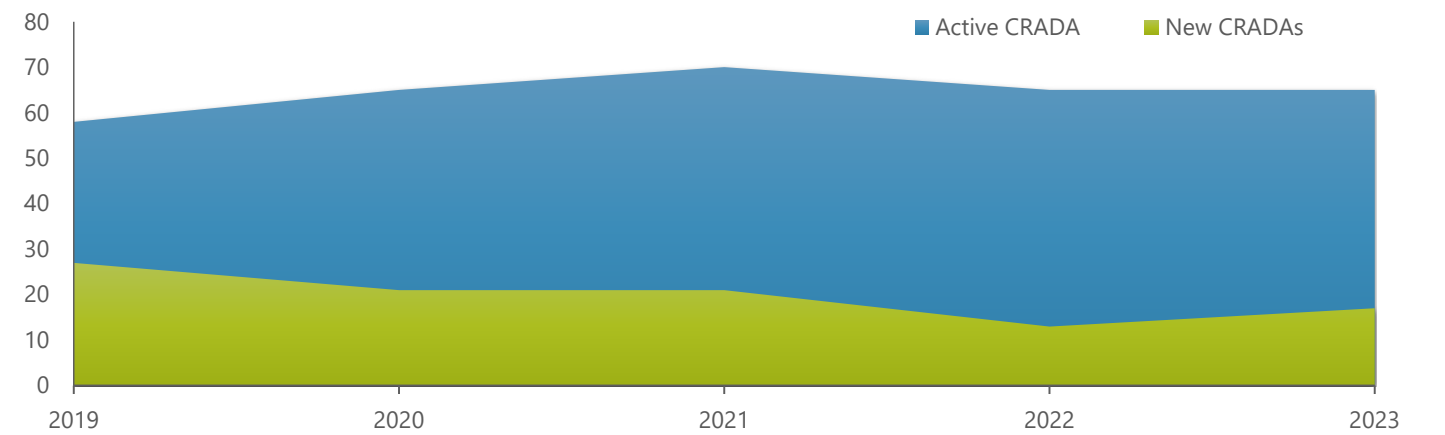


COPYRIGHTS



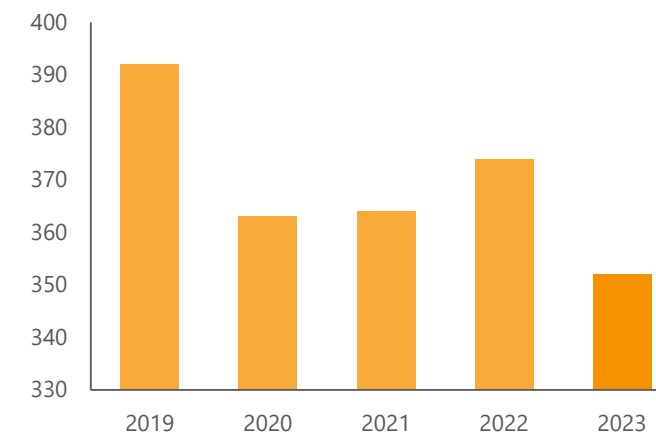
LLNL obtained more than 350 copyright assertions from 2019 to 2023, helping to protect the Laboratory's intellectual property.

CRADA AGREEMENTS



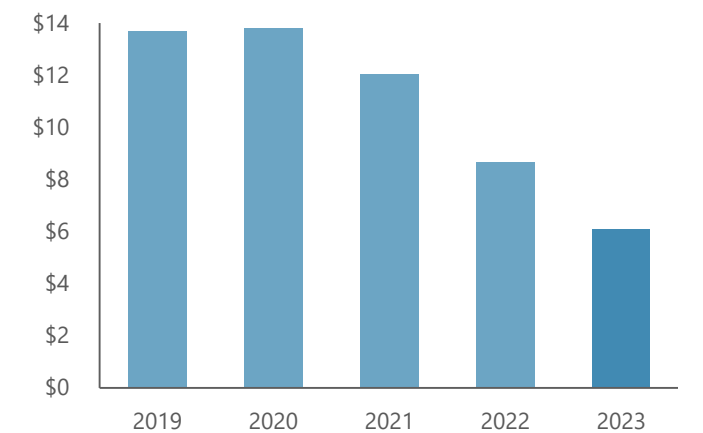
ACTIVE COMMERCIAL LICENSES

LLNL has maintained over 350 active commercial licenses annually from 2019 to 2023.



CRADA PARTNER FUNDS TO LLNL (\$ MILLIONS)

These funds play a key role in our technology transfer activities.



INNOVATION & PARTNERSHIPS OFFICE **OPERATIONS**

Optimizing the Technology Transfer Process

IPO OPERATIONS | BETTER, STRONGER, FASTER

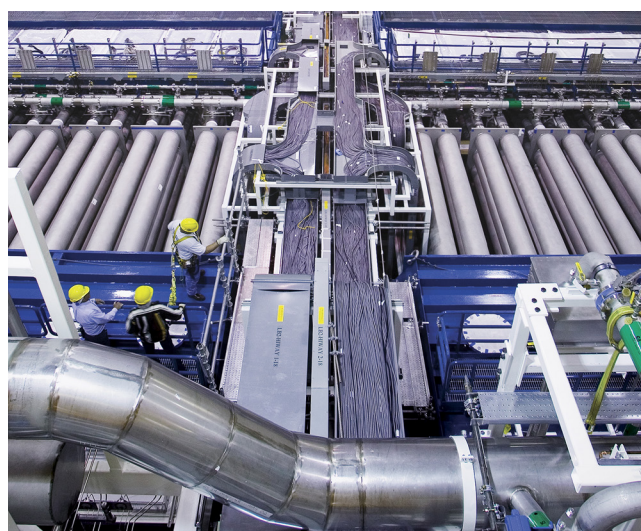
While metrics such as the number of partnership agreements or licenses negotiated serve as direct indicators of IPO's success in transferring technology from LLNL to the private sector, they are the end-goals—a culmination of the many contributing activities in earlier stages of the technology transfer pipeline. If these activities can be performed more efficiently, the number of partnerships and licenses will naturally increase.

In FY23, the IPO Team embarked on streamlining operations that ranged from small steps such as creating new fillable forms to overhauling the process of marketing LLNL technologies. The main impetus for these changes originated when the decision was made to update the intellectual property management software. The new, more advanced platform will be able to manage the complete tech transfer lifecycle from disclosure to commercialization. It will be a considerable upgrade from the rigid database that the Team has been using for the past 20 years, but are now struggling to use effectively. The team is excited to transition to the new platform in FY24.

MARKETING LLNL TECH, IMPROVED WORKFLOW

The IPO Team is undertaking a monumental effort to streamline its patent filing decision process. One part of the process is the public posting of LLNL's licensing opportunities. To meet DOE's Fairness of Opportunity Order, IPO is required to take all reasonable measures to broadly notify interested external parties of LLNL technologies available for transfer through licensing or collaborative arrangements.

As with many national laboratories, before any technology-related content can be posted publicly, it must be reviewed and released by the Laboratory. To accelerate the review and posting process, a new Technology Outreach Form (TOF) was developed. Once released, the information within the TOF is then published on multiple outreach platforms including IPO's external website, the U.S. government's System for Award Management (SAM.gov), and DOE's Laboratory Partnering Service, allowing IPO to satisfy the Fairness of Opportunity requirements.



One of NIF's two identical laser bays; each bay has two clusters of 48 beamlines, one on either side of the utility spine running down the middle of the bay (Jacqueline McBride).

NEW ONLINE FORMS & AGREEMENT TEMPLATES

While working to bring the new IP management platform online, the IPO Team also investigated other new digital tools for improving operational efficiency in the tech transfer pipeline. One example is the creation of an online form for routine due diligence research requests. These requests are required to assess companies for foreign affiliations and gather other information that may impact the decision to work with the potential partner.

Another change to the pipeline is the update of agreement templates. In addition to creating a repository and updating the standard agreement templates, in FY23, IPO crafted and executed its first Master Scope of Work Cooperative Research and Development Agreement (MSW CRADA) with ATOM Research Alliance. Since this agreement has been approved by DOE Headquarters, any future MSW CRADA will not need approval, thus opening new ways of working with the private sector.

IPO **TEAM**

New Staff



MATT GARRETT

DIRECTOR

Matt joined LLNL as the Director of the IPO in May 2023. Prior, Matt served as Chief Technology Officer and Director of Technology Transfer & Private Partnerships at SLAC National Accelerator Laboratory, managed and operated by Stanford University. Before working at SLAC, Matt served as Commercialization Manager in the Technology Transfer Office at Oak Ridge National Laboratory.

Matt holds an M.S. in Chemistry from The Pennsylvania State University and a B.S. in Chemistry from Florida State University.

TIMINA WALTON

ADMINISTRATIVE SPECIALIST

Timina joined IPO in July 2023 as the Administrative Specialist. Timina has over 10 years executive administrative experience working with fast moving teams in the Bioscience, Healthcare, and Consumer Packaged Goods industries. Prior to joining the team, she worked at The Clorox Company.

SAMANTHA MADRU

AGREEMENTS SPECIALIST

Samantha joined the Innovation and Partnerships Office team in Spring 2023. Prior to joining LLNL, Samantha worked for California Business Escrow as a Jr. Escrow Officer. Samantha studied Business Administration at Modesto Junior College and graduated with an Associate's Degree in Business Administration.



JARED LYNCH, PHD

BUSINESS DEVELOPMENT EXECUTIVE

Jared joined IPO in May 2023 as the Business Development Executive responsible for the commercialization of technologies and management of intellectual property within Chemicals & Materials as well as Energy & Environment portfolios. Prior to joining LLNL, Jared worked in startup companies that focused on biomaterials as well as quantum dot technology.

He received his B.S. in Chemistry from Florida State University, and his Ph.D. in Analytical Chemistry from University of Florida.



CHARLOTTE ENG, PHD

BUSINESS DEVELOPMENT EXECUTIVE

Charlotte joined in October 2022 as a Business Development Executive responsible for designing informational materials and researching industry partners aligned with the various LLNL technology portfolios. Prior to joining IPO, she was a forensic microscopist at LLNL. Before working at the Lab she was the senior Art Conservation Scientist at the LA County Museum of Art.

She received her Ph.D. in Materials Science & Engineering from Stony Brook University.

JOE CORRALES

BUSINESS ANALYST

SONAL GADRE

INTELLECTUAL PROPERTY SPECIALIST

MEL HENNING

BUSINESS ANALYST



Photo top
National Lab Accelerator Pitch Event | co-hosted by SLAC and LLNL, November 16, 2022 (Hannah Farquar).

Photo right
Energy I-Corps Cohort 17, mid-September 2023 (Kira Vos, Department of Energy, Office of Technology Transitions).

Photo far right
Finalists and Winners of the 2023 R&D 100 Awards (Mark Gartland).



CELEBRATING LLNL INNOVATORS

Entrepreneurship Programs

LLNL entrepreneurial training programs have been incredibly successful in commercializing technology developed at the laboratory! Here are some highlights for FY23:

- The National Lab Accelerator Program, described as a "Shark Tank" for Department of Energy National Lab researchers, had nine participants this year.
- For their efforts in coordinating the National Lab Accelerator Program, IPO Team members Hannah Farquar and Roger Werne received the 2023 "Best in Class for Innovative Technology Transfer" and the DOE Office of Technology Transitions (OTT) Director's Award!
- Thirteen LLNL researchers participated in the National Labs Entrepreneurship Academy (NLEA). This program was started by LLNL in 2015 and has since trained 240 LLNL plus 124 Sandia National Laboratories researchers.
- Two LLNL teams were trained this year for Energy I-Corps; one was selected to join ten other National Lab teams to form this year's Cohort 17.

2023 R&D 100 FINALIST
DSRD vapor deposition process creates powerful electrical components

2023 R&D 100 WINNER
PB-UHF enables data monitoring through containment walls

2023 R&D 100 WINNER
CANDLE leverages machine learning to accelerate cancer research

2023 R&D 100 WINNER
Variorum measures and optimizes supercomputer performance

zfp saves storage, time, and compute power with flexible data compression

Making the impossible possible
Experiments at LLNL's National Ignition Facility in December 2022 and July 2023 resulted in ignition, in which the energy produced from a fusion reaction exceeds that required to spark the reaction.

llnl.gov

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27944. LLNL-MI-855191

Award Winners

In August 2023, the trade journal R&D World Magazine announced the 2023 winners of the R&D 100 awards, often called the "Oscars of innovation," recognizing new commercial products, technologies, and materials that are available for sale or license for their technological significance. LLNL scientists and engineers netted three awards among the top 100 inventions worldwide.

In 2023, LLNL R&D 100 awards include a software suite that helps apply deep-learning techniques to major science and data challenges in cancer research (CANDLE); software that helps better understand the power, energy and performance of supercomputers (Variorum); and a number format that permits fast, accurate data compression for modern supercomputer applications (ZFP).

All three of LLNL's R&D 100 award winners received internal "seed money" from the Laboratory Directed Research and Development program. This funding enables the undertaking of high-risk, potentially high-payoff projects at the forefront of science and technology.

ZFP was developed by a team of LLNL researchers led by computer scientist Peter Lindstrom and computer scientists Danielle Asher and Mark C. Miller. In addition, three former Lab employees were part of the team: Stephen Herbein, Matthew Larsen, and Markus Salasoo.

The Variorum team is led by Lab computer scientist Tapasya Patki and includes computer scientists Aniruddha Marathe, Barry Rountree, Eric Green, Kathleen Shoga, and Stephanie Brink.

The CANDLE collaborators are: Argonne, Oak Ridge, Lawrence Livermore, and Los Alamos national laboratories, as well as Fredrick National Laboratory for Cancer Research. The LLNL part of the ECP-CANDLE team is led by Lab computer scientist Brian Van Essen and chief computational scientist Fred Streit. The team also includes Tom Benson, Adam Moody, Tal Ben-Nun, Nikoli Dryden, and Pier Fiedorowicz as well as former Lab employees David Hysom, Sam Ade Jacobs, Naoya Maruyama, and Tim Moon.

SUCCESS STORY IGNITING CHANGE

Business Development Executive: Dave Dawes (retired)

Agreement and IP Specialists: Connie Pitcock (retired), Alicera Aubel, Terry Contreras

On December 5, 2022, the LLNL team at the National Ignition Facility (NIF) fired 192 laser beams into a hohlraum that housed a capsule containing partially frozen hydrogen isotopes. The result was fusion ignition—producing more fusion energy than the amount of laser energy delivered to the NIF target. The experiment delivered 2.05 megajoules (million Joules or MJ) to the target and produced 3.15 MJ of energy. LLNL has been working toward ignition since the 1960s when physicists realized lasers could spark a fusion reaction and that inertial confinement fusion (ICF) by lasers could be used for commercial power generation and for research enabling nuclear weapons stockpile stewardship. Since the first ignition, NIF has conducted three more successful shots and expanded the possibilities for ICF and commercialized fusion energy. These achievements set the stage for LLNL to build on its technology transfer successes in the field of fusion.

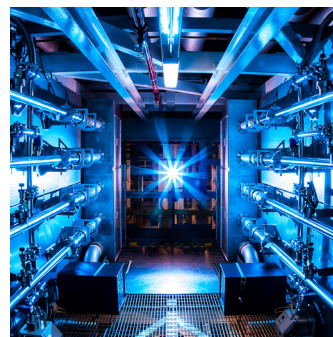
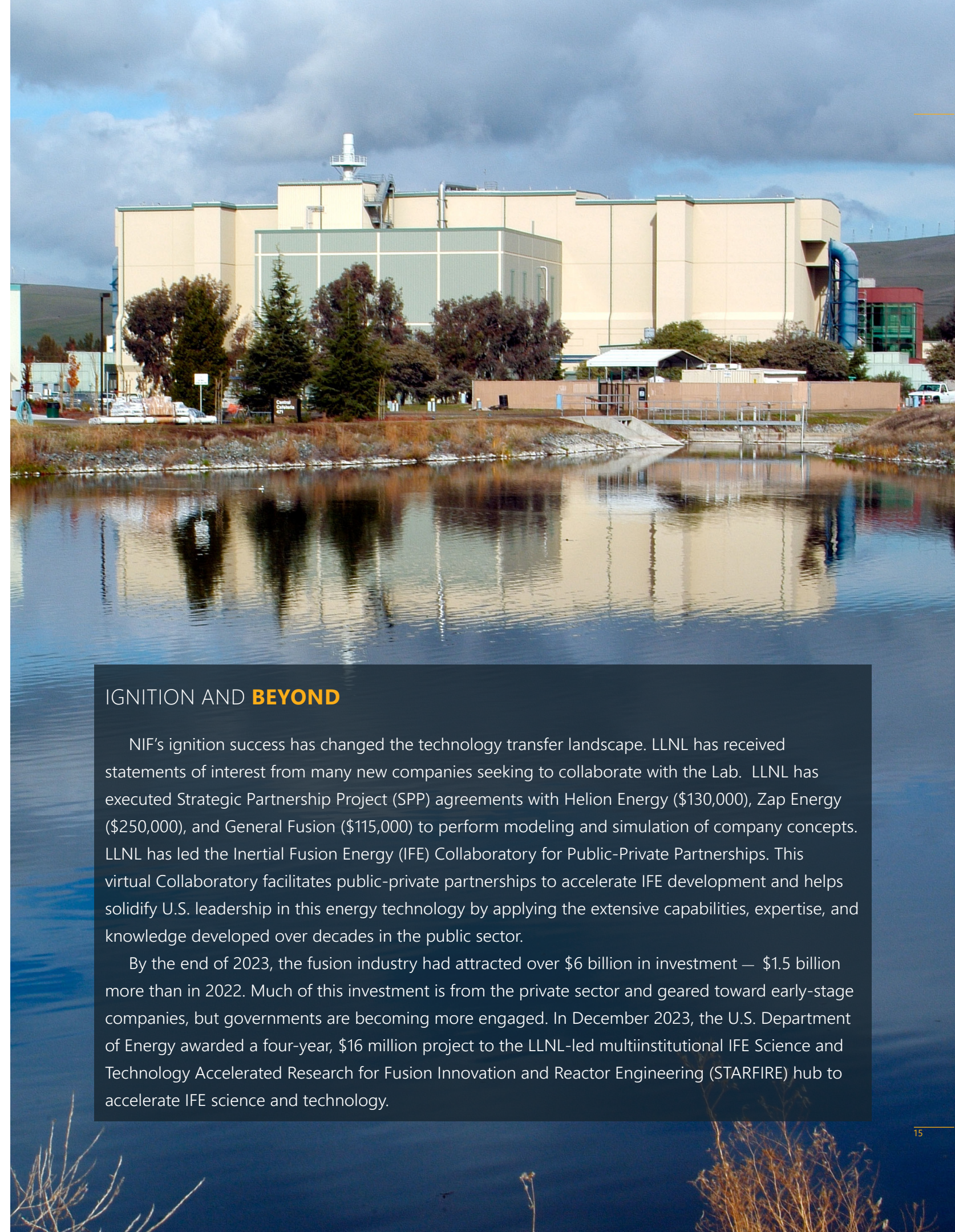


Photo left page

A color-enhanced image of the inside of a NIF preamplifier support structure (Damien Jemison).

Photo right page

National Ignition Facility (NIF) by the lake (Patty Santos & Tom Reason).



LLNL's Innovation and Partnerships Office (IPO) has supported fusion researchers from the beginning to build the necessary research facilities, such as NIF, and to commercialize laser and optics technologies. Before research could be conducted, complex infrastructure and laboratory space had to be in place. LLNL looked to the private sector for companies to deliver what was required, a challenge given how confidential and technical the design specifications were. IPO facilitated procurement of the necessary building and laboratory equipment through nondisclosure agreements (NDAs) that gave the businesses the information they needed to build and outfit the research spaces without sharing details of the work being done. Many companies have partnered with LLNL since the Nova Laser Fusion Facility, which predates NIF, and have evolved their own capabilities in tandem with the development and launch of NIF. These include Zygo, Corning, and SCHOTT, while other companies such as Bond Optics, L3Harris, Sydor Optics, Spectra Physics, and more joined later in NIF's evolution. Maintaining those enduring business relationships has been a key priority for IPO.

In addition, NIF laser and optics technologies have yielded over 250 issued patents and patent applications (all processed through IPO or its technology transfer predecessors). IPO managed the Laser Inertial Fusion Energy (LIFE) portfolio of technologies used not only at NIF but in Cooperative Research and Development Agreements (CRADAs) as well as Licensing and ACT agreements with industry partners.

IPO helped protect and facilitate development of the unique materials and components necessary to meet NIF's fusion goal. In 2017, IPO processed a CRADA with Electro-Optics Technology (now Coherent) to collaborate with LLNL researchers on the development and manufacture of a 100-kW Faraday rotator for high-powered laser systems. Coherent now supplies NIF with wedge-focused lenses used in NIF's Final Optics

Assembly to focus the laser beams onto the target.

Moreover, IPO recognized that the market for fusion is very small and to make greater impact beyond supporting NIF goals, LLNL technologies should be applied to broader industry sectors — perhaps those that would benefit from improved lasers and optics. An exemplar of this is laser peening, the use of intense laser light to improve the reliability of a material, which has also been a tech transfer success for IPO. Since LLNL's 2003 CRADA with the Metal Improvement Company (MIC), laser peening technology has been a primary tool to treat and improve flight vehicle materials. To date, laser peening has generated the third-highest amount of royalties of LLNL's licensed technologies.

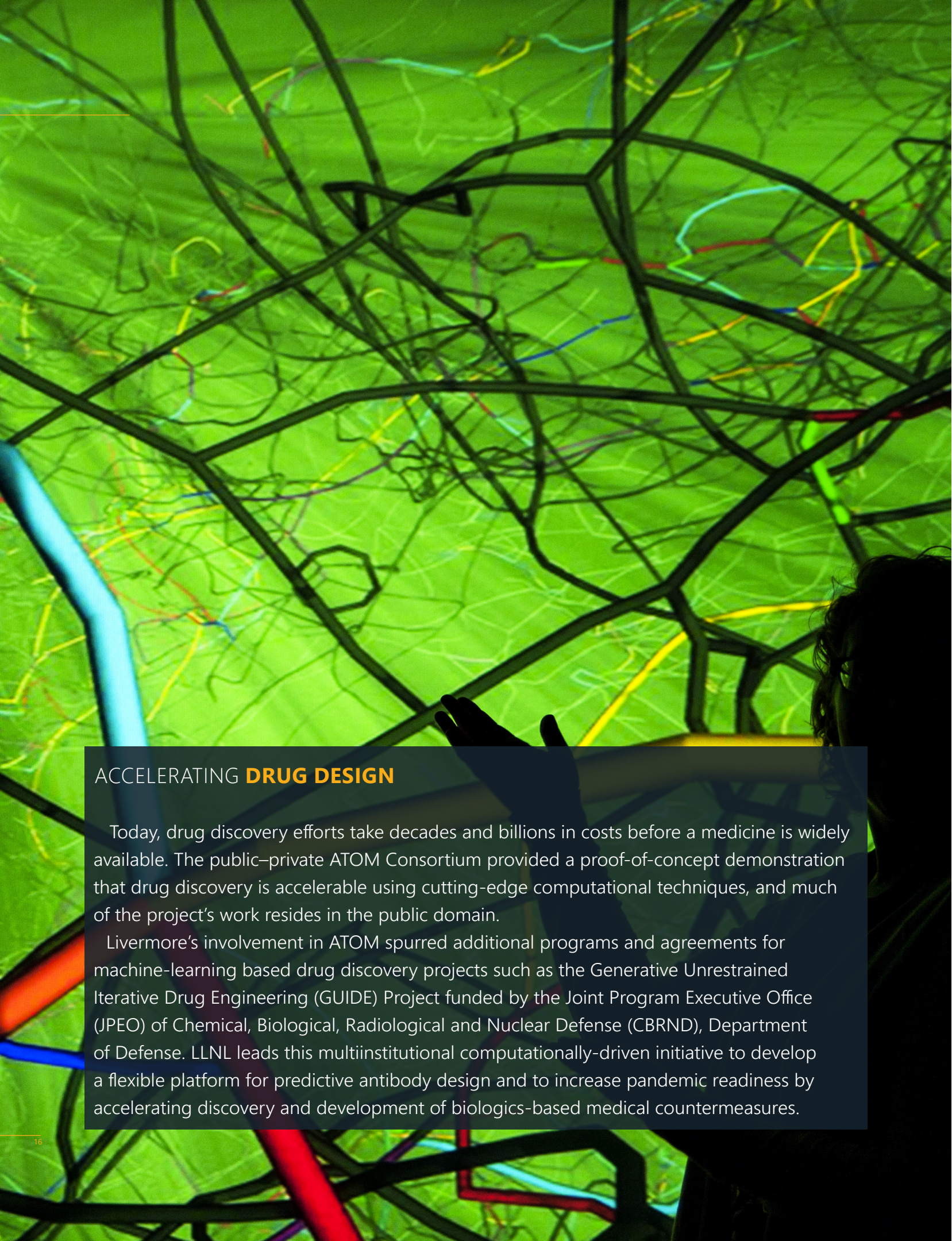
Another transfer success is IPO's licensing of LLNL's diode-based additive manufacturing (DiAM) technique to Seurat Technologies. Using the Lab's DiAM method, the company developed their Large-Area laser Powder Bed Fusion technology. This technology allows them to flash 3D print large areas of metal powder and manufacture more complex metal structures for different industrial uses more quickly and more cost effectively than with traditional casting and forging techniques. Following LLNL's licensing of the DiAM technology to Seurat in 2016, the company has since secured investment from several global companies.

The high-repetition-rate advanced petawatt laser system (HAPLS), designed by LLNL, will contribute to new schemes for ICF including shock ignition and fast ignition. It also has applications in astrophysical phenomena, and provides sophisticated diagnostic tools for high-energy density physics plasma research. HAPLS won a regional award for technology transfer from the Federal Laboratory Consortium (FLC) in 2018, and LLNL and Lasertel, Inc. won a 2015 R&D 100 Award for the high-power intelligent laser diode system, a key component of HAPLS.

IGNITION AND BEYOND

NIF's ignition success has changed the technology transfer landscape. LLNL has received statements of interest from many new companies seeking to collaborate with the Lab. LLNL has executed Strategic Partnership Project (SPP) agreements with Helion Energy (\$130,000), Zap Energy (\$250,000), and General Fusion (\$115,000) to perform modeling and simulation of company concepts. LLNL has led the Inertial Fusion Energy (IFE) Collaboratory for Public-Private Partnerships. This virtual Collaboratory facilitates public-private partnerships to accelerate IFE development and helps solidify U.S. leadership in this energy technology by applying the extensive capabilities, expertise, and knowledge developed over decades in the public sector.

By the end of 2023, the fusion industry had attracted over \$6 billion in investment — \$1.5 billion more than in 2022. Much of this investment is from the private sector and geared toward early-stage companies, but governments are becoming more engaged. In December 2023, the U.S. Department of Energy awarded a four-year, \$16 million project to the LLNL-led multiinstitutional IFE Science and Technology Accelerated Research for Fusion Innovation and Reactor Engineering (STARFIRE) hub to accelerate IFE science and technology.



ACCELERATING DRUG DESIGN

Today, drug discovery efforts take decades and billions in costs before a medicine is widely available. The public-private ATOM Consortium provided a proof-of-concept demonstration that drug discovery is accelerable using cutting-edge computational techniques, and much of the project's work resides in the public domain.

Livermore's involvement in ATOM spurred additional programs and agreements for machine-learning based drug discovery projects such as the Generative Unrestrained Iterative Drug Engineering (GUIDE) Project funded by the Joint Program Executive Office (JPEO) of Chemical, Biological, Radiological and Nuclear Defense (CBRND), Department of Defense. LLNL leads this multiinstitutional computationally-driven initiative to develop a flexible platform for predictive antibody design and to increase pandemic readiness by accelerating discovery and development of biologics-based medical countermeasures.

SUCCESS STORY ATOM CONSORTIUM

Business Development Executive: Yash Vaishnav
Agreement Specialist: Tami Plisco

Drug development often requires over a decade and billions of dollars to realize a safe, viable, economical product. Initial drug discovery requires roughly one-third of available drug development resources, and only around 12% of proposed medicines ever experience clinical success. From millions of conceivable molecules, thousands of promising candidates must be screened, structurally optimized, and tested in preclinical trials before advancing to human clinical trials. These challenges of scale are best addressed by high-performance computing (HPC) tools.

The computing-centered drug discovery framework developed by the Accelerating Therapeutics for Opportunities in Medicine (ATOM) Consortium drastically compresses the drug discovery timeline. ATOM succeeded in discovering an efficacious, biologically mediating agent in under one year by combining academic expertise, industrial experience, and national computing resources. ATOM's open-source platform for active-learning based generative design and optimization of drug molecules rapidly explores chemical spaces with growing predictive accuracy.

ATOM provides a multiparameter molecule design and testing platform to accelerate the iterative lead discovery phase of drug development. The platform uses machine learning (ML) to generate, screen, and predict clinical efficacy of novel molecules, preserving resources otherwise spent on research dead ends and duplicating unpublished studies. Underpinning the platform is the ATOM Modeling Pipeline (AMPL), housing generative and predictive ML tools to estimate molecules' clinical efficacy based on structural properties, molecular dynamics simulations, and experimental results. The framework intakes tested molecules by employing graph convolution and molecule fingerprinting to encode structure, then analyzes chemical properties to predict clinical efficacy, human safety, pharmacokinetics, and other related measurements.

Critically, AMPL identifies when more information is necessary to improve property prediction. Gaps are filled by molecular dynamics simulations and results of in vitro or in vivo experiments, growing AMPL's working compound library and refining property predictions. Yet, many innovative molecules remain to be synthesized or tested, and academic publications—some unpublished—contain troves of data inaccessible to researchers. ATOM provides the pathway for integrating existing and forthcoming data.

The ATOM Consortium was founded in 2017 by LLNL; the Frederick National Laboratory for Cancer Research; the University of California,

San Francisco (UCSF); and pharmaceutical company GSK (formerly GlaxoSmithKline). The same year, LLNL's Innovation and Partnerships Office (IPO) processed the Cooperative Research and Development Agreement (CRADA), which was subsequently executed by the founding partners. In 2021, Argonne, Brookhaven, and Oak Ridge national laboratories joined the ATOM Consortium and ATOM CRADA, with LLNL serving as a lead entity for both.

Public-private partnership enabled national-level entities to benefit from private pharmaceutical experience, and supported the building of ATOM's pre-competitive platform. Livermore provided world-class supercomputing resources and expertise in data science, cognitive and parallel computing, and ML algorithm development. Private sector partners leveraged experience in drug discovery, synthesis, and clinical testing. GSK supplied data on approximately three million unused pharmacological compounds instrumental to constructing and running AMPL.

The ATOM Consortium regularly published research and released open-source resources, including: an open-curated, model-ready molecule library; the aforementioned AMPL; the Livermore Big Artificial Neural Network (LBANN) Toolkit, a computing platform for generative molecular models; and Generative Molecular Design (GMD), an HPC platform for parallel optimization of efficacy, safety, and pharmacokinetics. Having achieved its one-year target-to-candidate molecule goals, the ATOM Consortium expired in 2022. Its legacy continues as the ATOM Research Alliance (ARA), a 501(c)(3) nonprofit organization with whom LLNL entered into a Master Scope of Work CRADA in 2022 to expedite research. ARA maintains adaptable mechanisms to support individual researchers, molecule discovery technologies, and biotechnology investors to protect intellectual property and fulfill ARA's drug discovery democratization obligations.

Photo left page

Power Wall used for viewing high-resolution images and data comparisons (LLNL).

Photo right page

Logo for Accelerating Therapeutics for Opportunities in Medicine (ATOM) consortium.



SUCCESS STORY GEOS & PROJECT FC-MAELSTROM

Business Development Executive: Dave Dawes (retired)

Digital Assets Coordinator: Mary Holden-Sanchez

Agreement Specialists: Alicera Aubel, Connie Pitcock (retired)

To meet national climate goals, underground sequestration is a promising tactic to mitigate atmospheric carbon. Identifying ideal sites and studying long-term effects of storage is therefore crucial. Scientists at Lawrence Livermore collaborated with university and industry partners to develop GEOS, an open-source reservoir modeling and simulation tool that unifies mechanical engineering, seismology, hydrology, and computational geosciences understanding.

To perform carbon sequestration—the original motivation for GEOS’s development—carbon dioxide is first captured from the air or directly from emissions sources. The collected material is compressed into a liquid state and injected kilometers below ground into naturally occurring reservoirs. Injection is far from haphazard; geologic structure must be confirmed physically and chemically resilient to an enormous influx of foreign material—a challenging feat considering reservoirs are obscured by kilometers of earth. Modeling and simulation is thus essential for such assessments.

GEOS integrates scalable multiphysics algorithms to simulate reservoir performance across large spatial and temporal scales. For carbon sequestration, GEOS uses mathematical models of geologic structure to simulate the physical and chemical effects of carbon fluid injection on a site-by-site basis. For other infrastructure projects, GEOS’s governing fluid dynamics, thermodynamics, and other physical parameters can be set to reflect the properties of other substances, such as hydrogen. Because not all potential users have cutting-edge computing power, the tool is executable on personal computing and supercomputing systems alike. GEOS is currently running on Oak Ridge National Laboratory’s Frontier exascale computer and will also run on LLNL’s El Capitan.

GEOS development partners TotalEnergies and Stanford University are no strangers to collaborating with LLNL on subsurface modeling technologies, having previously carried out multiple related projects. As earlier efforts concluded, enduring mutual interests in geologic carbon storage, software development, and HPC spurred yet another Collaborative Research and Development Agreement (CRADA), this time with the aim of consolidating these capabilities into a single, open-source tool.

Developing and refining GEOS codes was possible due to the complementary strengths of each research partner. Livermore

brought expertise in geomechanics, simulator development, and high performance computing broadly. Stanford University and TotalEnergies both have significant background in reservoir simulation, with Stanford leaning towards simulator development and TotalEnergies bringing decades of industrial field experience.

Finalizing agreement language required extensive discussions of intellectual property rights and how to provide open-source software deliverables. LLNL’s Innovation and Partnerships Office (IPO) negotiated a complex CRADA agreement—including a foreign partner review—and shepherded the arrangement through the Department of Energy’s elaborate approval processes. Copyright ownership was granted equally to each collaborator regardless of individual code contributions. The code license was decided as open source under an LGPL version 2.1 license; commercial products could still be developed using its library, so long as it is called dynamically. Funding for research collaboration was provided by the DOE Exascale Computing Project through the Exascale Subsurface Simulator Project, and by TotalEnergies via the FC-MAELSTROM Project.

Public-private partnership successfully delivered a next-generation reservoir simulation framework for CO₂ storage and beyond. GEOS’s open source code allows operators to model reservoir systems with greater spatial resolution and physical fidelity than ever before while avoiding the steep commercial licenses common in competing tools. The effort rapidly transformed academic concepts of subsurface physics modeling into industrial applications with increased technology readiness levels. In fact, some CO₂ storage projects planned using GEOS have already launched.

GEOS development remains ongoing. The team recently began a Phase 2 CRADA, adding Chevron to the partnership and expanding GEOS’s modeling capabilities for further geoscience phenomena such as subsurface hydrogen storage and geothermal energy.

Photo left page

A simulation of the fluid pressure distribution in a faulted reservoir (geologic data courtesy Gulf Coast Carbon Center) due to CO₂ injection through multiple wells (LLNL).

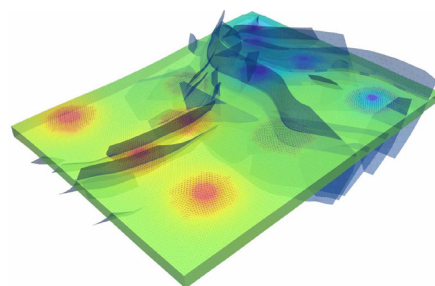
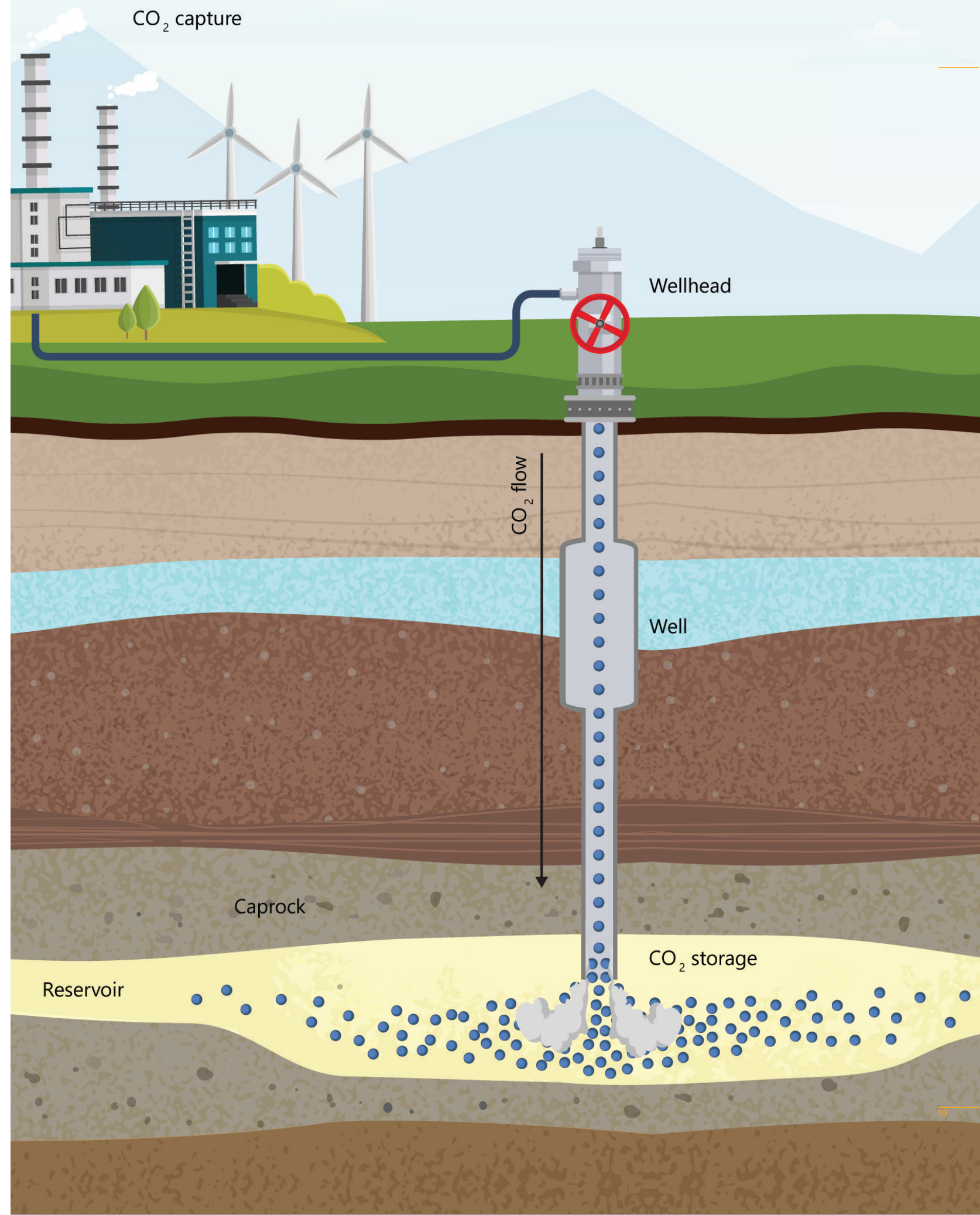
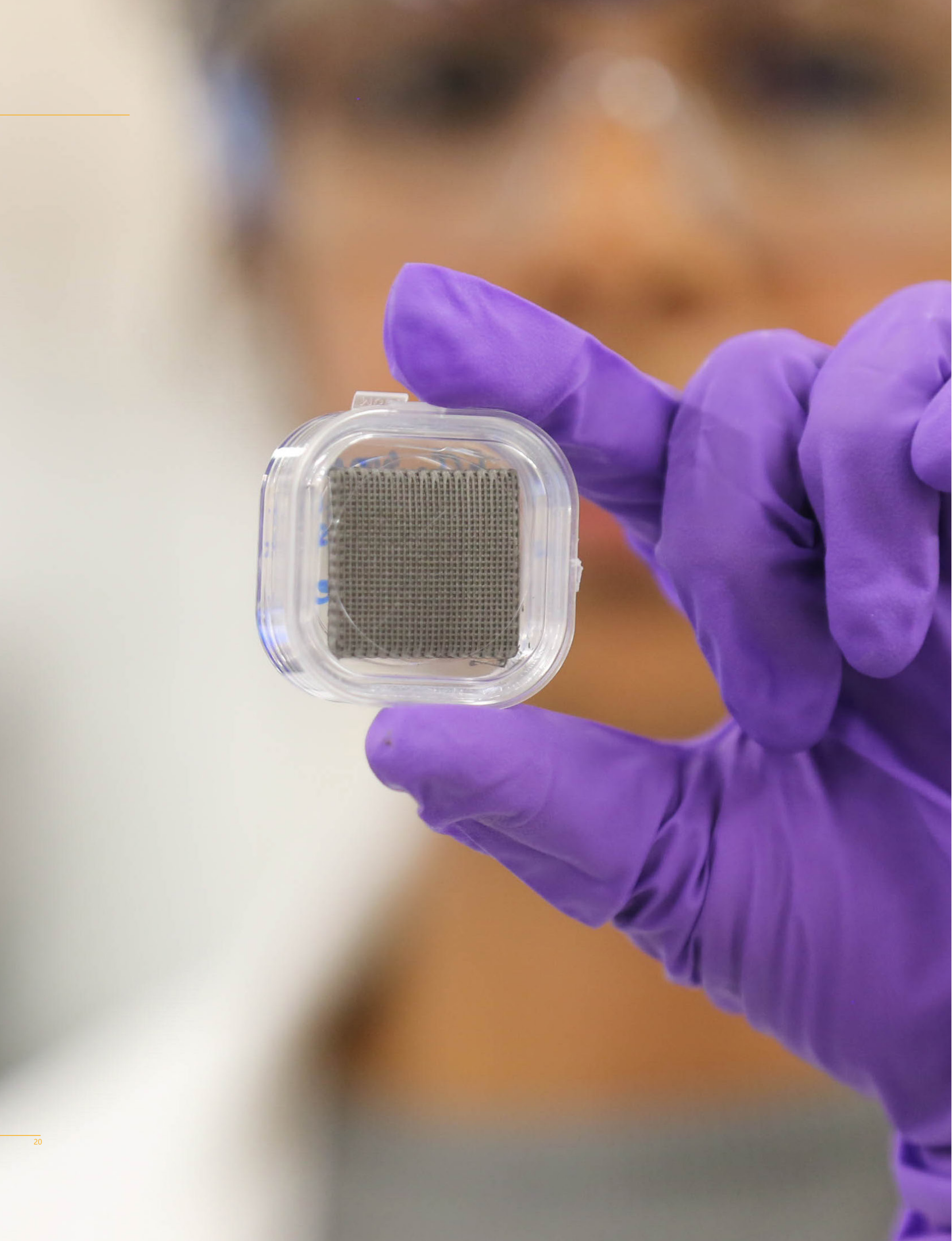


Photo right page

Illustration of the process of injecting compressed liquid carbon dioxide into an underground reservoir (LLNL).





SUCCESS STORY

ENERGY INKS

*Business Development Executive: Genaro Mempin
Agreement Specialist: Alicera Aabel*

Energy Inks, 3D printing feedstock inks developed by LLNL researchers, are primed to revolutionize 3D printing capabilities on a global scale. These ink products can enable 3D-printing of functional battery and supercapacitor components, sensors, and other devices more efficiently than traditional manufacturing. “To fabricate parts from a variety of materials, each ink was tailored to deliver the optimal combination of properties,” says LLNL scientist Swetha Chandrasekaran, one of the inventors of Energy Inks. “Controlling the composition and rheological behavior of the feedstock inks was crucial to forming self-supporting filaments that maintain their shape as they span over previously deposited layers.” Through an LLNL–MilliporeSigma partnership, three different Energy Inks formulations have been introduced to the market.

MilliporeSigma, a global life science and industrial and lab chemicals company, saw Energy Inks’ potential early in their development and contacted LLNL to develop the technology further. In 2020, LLNL’s Innovation and Partnerships Office (IPO) licensed the technology to MilliporeSigma and executed a Cooperative Research and Development Agreement (CRADA) with the goal of reaching academic and commercial partners who would use the specialized inks in their work. To increase ink production and reach a wider customer base, the team secured a Department of Energy (DOE) Technology Commercialization Fund (TCF) grant to fund product development.

LLNL researchers and technology transfer professionals acknowledged that commercializing a materials innovation would be a challenge; the inks needed to be optimized and analyzed for stability—specifically, a shelf life of at least ten months—to be included in the MilliporeSigma product catalog. LLNL scientist Alyssa Troksa worked with MilliporeSigma to achieve this optimization in one of the inks. “We tuned the relative concentrations of nanoparticles and polymer binders and adjusted storage conditions and mixing procedures until we found a formulation best suited for printing and energetic performance,” says Troksa.

The team also understood that any optimization challenges would be rewarded by the opportunities provided by Energy Inks, both in revolutionizing the 3D-printing market and enabling more efficient energy device production to meet an increasing global demand. To increase adoption and penetrate the market, the team developed an ongoing model using MilliporeSigma’s reach of 1.6 million annual customers and distribution sites in 66 countries to sell Energy Inks to universities and commercial companies. Customer feedback was considered alongside LLNL’s materials expertise to iteratively improve formulations and adapt them to real-world applications. This unique technology transfer has ensured that the Energy Inks technology

Photo left page

Swetha Chandrasekaran holding a 3D-printed graphene aerogel supercapacitor (Julie Russell).

Photo right page

Direct ink writing, a 3D printing process, uses high concentration graphene oxide ink to print aerogel electrodes (Julie Russell).



meets varying needs across a global audience.

The MilliporeSigma product line includes the following Energy Ink formulations, which feature long shelf-lives and high viscosity: 3D Printable Graphene Oxide Ink, 3D Printable Yttria Stabilized Zirconia Ink, and 3D Printable Ultra-High Temperature Boron Carbide Ink. The Energy Inks team has earned several awards for the technology, including a 2022 R&D 100 Award and a 2023 LLNL Physical and Life Sciences Scientific and Technical Award. Also in 2023, the Federal Laboratory Consortium (FLC) named the technology transfer effort Best in Region (Far West). The LLNL-MilliporeSigma team has raised awareness of Energy Inks through extensive outreach including MilliporeSigma’s online Technology Spotlight marketing platform, social media videos, and customer-facing slides highlighting each formulation.

The collaboration stands out by having improved a variety of technologies with one line of materials compared to a traditional technology transfer model of licensing, for example, a single new energy storage device or commercializing only one product at a time. Energy Inks can be applied to consumer electronics, transportation, and medical devices, making them a powerful tool to both conceive new energy technologies and expand upon existing ones.

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The easy availability of Energy Inks offers the potential to revolutionize how researchers design and test the next generation of alternative energy generation and storage devices.

- Adam Raw, Head of Materials Science Research and Development at MilliporeSigma

SUCCESS STORY HYDROGEN STORAGE

Business Development Executive: Jared Lynch, Dave Dawes (retired)
Agreement Specialist: Alicera Aubel

As consumer demand increases for delivered goods and services, shipping companies seek transportation technologies to lower emissions and meet transportation mandates. Hydrogen fuel promises zero emissions but is difficult to store in the volumes required for longer-distance travel. LLNL has tackled this challenge to hydrogen-fuel adoption since the 1990s, pioneering cryo-compressed hydrogen (CCH₂) storage to increase storage volume. Collaborative research with Linde, BMW, and others led to hydrogen storage tank designs for consumer automobiles and improvements to significantly reduce hydrogen venting from storage tanks. An LLNL-led demonstration in a hydrogen-fueled Toyota Prius concluded with a successful, 650-mile driving test.

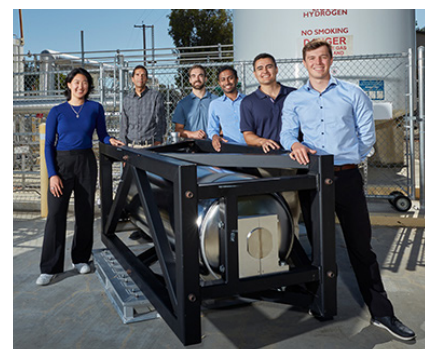


Photo left page
LLNL and Verne
researchers with
cryo-compressed
hydrogen storage
system (LLNL).

Photo right page
Bowdi Helgesen
loads a tank into the
pressure chamber
for testing (Blaise
Douros).

While past hydrogen fuel development efforts have focused on automotive applications, a partnership between LLNL and San Francisco start-up Verne has advanced the possibility of hydrogen-fueled commercial trucks for delivery and other industrial applications. Verne co-founders Ted McKlveen, David Jaramillo, and Bav Roy met as students and shared a vision of making hydrogen a viable fuel source. They built upon LLNL's foundational research to demonstrate that CCH₂ could decrease refueling time, expand driving range, and increase payload capacities of medium and heavy-duty trucks.

Companies such as Amazon and Caterpillar expressed interest in Verne's CCH₂ application. Investing in a new clean energy fuel system, however, represents a significant investment, even for industry leaders. Verne needed to test its modular CCH₂ storage systems, demonstrating their effectiveness for Class 8 vehicles—heavy-duty trucks that ship goods hundreds of miles at a time, through potholes and uneven pavement, in extreme heat, cold, and moisture, and across differing regional altitudes to safely reach their destinations.

Turning to the source of CCH₂ storage, Verne partnered with LLNL to assess the durability of CCH₂ tanks under typical operating conditions with an accelerated testing method. By reducing the time and resources required to prove tank performance, Verne could de-risk the technology quickly and draw commercial investment for pilot tests with Class 8 trucks.

Since the Verne-LLNL CCH₂ storage testing project supported United States goals for climate change mitigation, the partners applied for and received a Department of Energy (DOE) Technology Commercialization Fund (TCF) grant for \$192,000—matched with a \$295,000 investment from Verne.

The Verne-LLNL team of researchers at Livermore's Cryogenic Hydrogen Fueling Facility, led by mechanical engineer Nick Killingsworth, developed a multi-pronged approach that included sub-scale storage tank model fabrication and testing, accelerated fatigue testing, and extended CCH₂ cycling

testing. Working at LLNL's facilities provided Verne with a ready-made testbed, saving the startup the cost and risk of building its own testing infrastructure. The team ultimately tested a single-tank system storing more than 29 kilograms of CCH₂, significantly larger than previously demonstrated systems. Fabrication and testing of commercial-sized tanks will commence once enough data is obtained on the sub-scale tanks.

In addition to the TCF award, Verne secured a 24-month, \$500,000 Cooperative Research and Development Agreement (CRADA) through The Advanced Research Projects Agency – Energy (ARPA-E) in 2022 to continue work with LLNL. The Laboratory's Innovation and Partnerships Office maintained this important industry relationship while protecting LLNL's broader intellectual property, keeping a standard five-year protection period with the startup.

The follow-on partnership will build on the decades of LLNL's hydrogen storage research to lower costs and increase the operational flexibility of hydrogen fuel storage. The Verne-LLNL partnership moves the startup closer to its goal of zero-emission trucks traveling cross-country and through neighborhoods to meet the nation's delivery demands.

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Our solution builds upon decades of research pioneered at Livermore to provide a reliable, scalable, and cost-effective storage solution. We could not have done this without the team at Livermore. It's exciting to see this project head toward the commercialization phase where it can be adopted across the heavy-duty sector.

- David Jaramillo, co-founder of Verne





SUCCESS STORY

BIO ID

Business Development Executive: Yash Vaishnav
Agreement Specialist: Helen Peck (retired)

A small, portable device that can identify pathogens and viruses impacting humans, animals, and the environment sounds too good to be true. But research teams at Lawrence Livermore National Laboratory (LLNL) have designed, tested, and validated such a device. Over a decade ago, LLNL biomedical scientist Larry Dugan designed and tested Bio ID, a rapid and portable molecular diagnostics platform that can detect up to 20 target DNA or RNA sequences from one sample in 30 to 60 minutes using loop mediated isothermal amplification (LAMP) to detect pathogen nucleic acid.

Bio ID's original purpose was to enable the United States military to quickly detect biothreat agents in field and resource-constrained settings. With this purpose in mind, Dugan designed the diagnostic system to be small enough to fit in the palm of the hand and light enough considering the heavy loads military personnel regularly carry. The compact, portable device is rugged, easy to use, and allows for use in point-of-care, laboratory, field, and low-resource settings. The system is functional over temperatures ranging from -4°F to 113°F. Bio ID offers easy sample prep and colorimetric detection; different assay panels change color if there is a positive test, rendering identification of pathogens and viruses quick and easy for users.

In addition to military and low-resource settings, Bio ID's rapid diagnostics address human, animal, and environmental health and safety. Bio ID successfully identifies biothreat agents; human pathogens including E. Coli, pseudomonas, and Methicillin-resistant Staphylococcus aureus (MRSA); and foreign animal disease pathogens including foot and mouth disease. The technology offers improved diagnostic capabilities for urgent care, rural health facilities, and telemedicine and can be applied to point-of-care, clinical surveillance, and outbreak surveillance in the medical fields as well. Livestock owners can use Bio ID to rapidly detect and prevent endemic and epidemic disease outbreaks. Pet owners can conduct syndromic panels for common urinary and respiratory tract infections in companion animals, reducing diagnostic bottlenecks. Food growers, processors, and inspectors can use the system to detect microbial

Photo left page

Bio ID can provide on-site identification of microorganisms that are commonly responsible for corrosion in oil & gas operations.

Photo right page

Bio ID device, including the heater, cartridge, loading port, and lid (Larry Dugan).



contamination in food sources at different stages in the supply chain. Environmental quality organizations can use Bio ID to sample soil, air, and water. Depending on need, users can substitute their own proprietary assays into the device, and they can program Bio ID to meet specific requirements.

Recognizing Bio ID's potential in the diagnostics market, Dugan participated in LLNL's 2019 National Lab Accelerator, a six- to nine-month program that matches LLNL researchers with an experienced business mentor to help develop a technology's value proposition and business concept to pitch to the investment community. In 2021, Dugan partnered with a team of entrepreneurs in the National Nuclear Security Administration FedTech Startup Studio program—managed through LLNL's Innovation and Partnerships Office—that led to the founding of a startup company, BioVind, LLC by the entrepreneurs' team.

BioVind signed a Demonstration Agreement with LLNL in April 2022 to test the technology. In April 2023, BioVind signed an Option Agreement to evaluate the potential to commercialize the portable isothermal amplification device for detecting corrosion and biofouling-associated microbes found in oil and gas pipelines and storage. Although the Option Agreement does not allow BioVind to conduct activities for commercial development and sale of products until the option has been exercised for a commercial license, BioVind remains committed to developing the technology for commercial deployment. To date, the startup has received about \$1 million in grant funding from the California Energy Commission and \$50,000 in funding from SoCal Gas Company for testing and development.

**Lawrence Livermore National Laboratory's
Innovation and Partnerships Office**

IPO

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