Idaho National Laboratory ANNUAL REPORT FY 2014

# LDRD SNAPSHOT

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On the Cover Crystal boundaries could hold clues about nuclear fuel heat transfer. More on pg. 7.



## FROM THE DIRECTOR



John Grossenbacher Director, Idaho National Laboratory

## March 2015

It is my pleasure to present the Idaho National Laboratory (INL) fiscal year 2014 Laboratory Directed Research and Development (LDRD) Annual Report. This report demonstrates the types of cutting-edge research INL is undertaking to mature our technical capabilities and help ensure the nation's energy security. This is the third year we've produced the LDRD Snapshot to highlight the program's research diversity, university collaborations, metrics and successes.

INL's LDRD Program is operated in compliance with the Department of Energy (DOE) order 413.2B. This work aligns with INL's strategic plan and benefits the DOE. The program's diverse research and development emphasizes the DOE Office of Nuclear Energy (DOE-NE) mission, which encompasses both advanced nuclear science and technology, and underlying technologies. INL's LDRD program also advances that mission by helping develop technical capabilities necessary to support future DOE-NE research and development needs. Research areas during FY 2014 included reactor risk assessment and life extension, effects of storage and irradiation on nuclear fuel, fuel modeling, fuel recycling, and advanced radiation detection.

As a multiprogram national laboratory, INL research also serves the nation through technology that enhances homeland security. These research areas include wireless technologies, cybersecurity, electric grid reliability, nuclear nonproliferation and explosives protection. INL's isolated site and test bed infrastructure are ideal for experimentation and demonstrations that help protect the nation's resources and advance energy security.

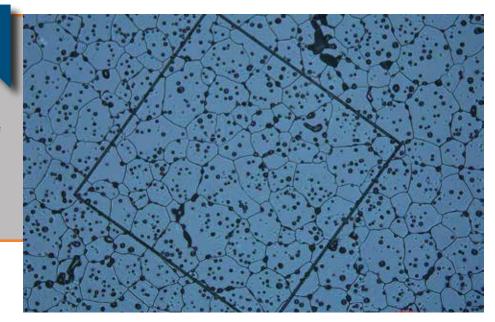
INL's science base is further strengthened by research to advance alternative energy systems that reduce greenhouse gas emissions and bolster energy security. INL's applied science and real-world assessments of improved energy systems and natural resource development help secure the country's future and protect the environment.

This year's LDRD projects offer a snapshot of the diverse creativity and expertise residing at INL. They offer innovative approaches to scientific questions and technical problems. In short, these projects help the lab maintain scientific and technical vitality, while fostering creativity and stimulating exploration at the forefront of science and technology.

I am proud of the accomplishments and opportunities that INL's LDRD projects provide to the nation. I encourage you to take the time to review these project narratives and reflect on their contributions.

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**On the cover** Fabricated pellets of a nuclear fuel surrogate (CeO<sub>2</sub>) enable researchers to study how characteristics at the "grain boundaries" between individual crystals of material impact heat transfer (project 13-105, led by Jian Gan). More on pg. 7.



## TABLE OF CONTENTS

Introduction: Mission and metrics of INL's LDRD program
<b>Research Project Highlights:</b> Brief descriptions of LDRD projects spanning the breadth of INL's research and development objectives
Awards & Recognition:LDRD researchers honored in FY 201414
University Collaborations: Overview of LDRD university interactions including collaborations, doctoral research projects, interns and postdoctoral fellows
<b>Project summaries:</b> Detailed descriptions of all FY 2014 LDRD projects, including those referenced by project number in this publicationCD, online

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## INTRODUCTION

## INTRODUCTION

The FY 2014 LDRD Annual Report Snapshot provides a glimpse of the diverse research performed to develop and ensure that INL's technical capabilities support current and future DOE and National Nuclear Security Administration (NNSA) missions and national priorities.

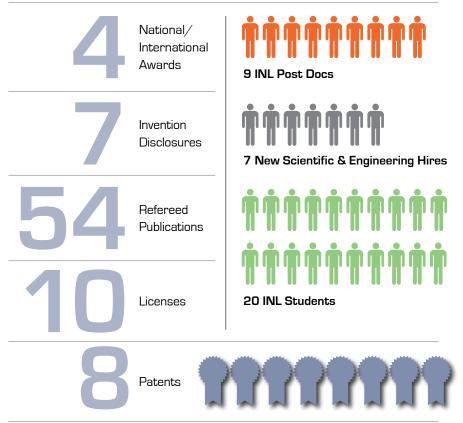
LDRD is essential, providing a means to maintain scientific and technical vitality by funding highly innovative, high-risk, potentially high-value research and development (R&D). INL's diverse LDRD portfolio explores scientific and engineering concepts to develop the needs of DOE's Office of Nuclear Energy (DOE-NE), including advanced reactor modeling, nuclear fuel advances, fuel recycling and nuclear nonproliferation. INL's LDRD research stimulates exploration at the forefront of cybersecurity, electric grid reliability and wireless technology. The forwardlooking nature of the laboratory's R&D strengthens the DOE mission by advancing hybrid energy systems and evolving energy needs.

The LDRD program proves its benefit each year through new programs, intellectual property, patents, copyrights, national and international awards, and publications. It also provides a means to feed the pipeline with scientists and engineers through undergraduate and graduate internships, postdoctoral assignments and internal Ph.D. candidates.

## **BENEFITS OF LDRD**

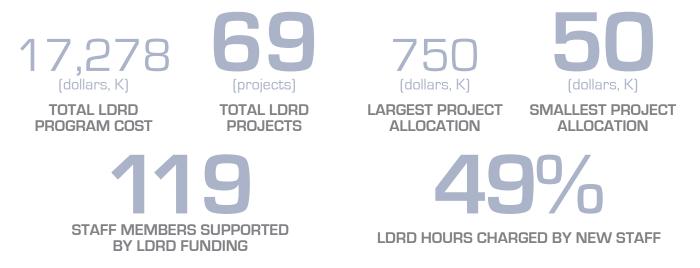
INL consistently realizes significant benefits from the LDRD program. The FY 2014 metrics are shown below.

## FY 2014 LDRD METRICS



INL's LDRD portfolio explores scientific and engineering concepts to stimulate exploration at the forefront of nuclear energy, national and homeland security, and energy security.

## FY 2014 LDRD PROGRAM STATISTICS



## **REPORT ORGANIZATION**

This report consists of the FY 2014 Annual Report Snapshot (Part I) and individual LDRD project highlights (Part II, via CD and online at www.inl.gov/LDRDINL). The Snapshot begins with research highlights that exemplify the diversity of scientific and engineering research performed at INL in FY 2014, followed by sections summarizing FY 2014 awards and recognition resulting from LDRD funding as well as university collaborations utilizing LDRD funding. Part II (CD) includes individual project summaries with a general description of the project, a summary of the scientific or technical progress achieved during the life of the project, a brief statement describing how the project benefited the DOE/NNSA missions, and relevant peer-reviewed publications and presentations. The CD also includes appendices (acronym list, author index and project relevance to DOE program offices) that may be useful to readers.

## THE LDRD PROCESS AT INL

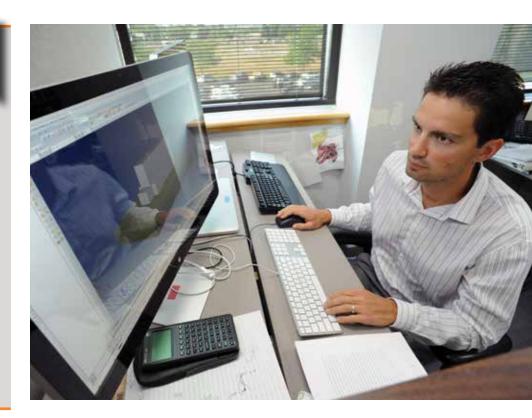
INL solicits ideas for LDRD projects through an annual call for proposals. The call takes into consideration the need to support key technical capability development, collaboration with university and industry partners, and crucial research that includes enabling or crosscutting science. These solicitations encourage innovative approaches proposed by individual researchers or small multidisciplinary teams.

The call for proposals includes a requirement for a pre-proposal followed by a full written proposal, a technical peer review and a management review prior to project selection. The intent of the preproposal process is to provide principal investigators the opportunity to briefly articulate an idea prior to investing time and effort to write a full proposal. The principal investigator for each selected project then submits a full detailed proposal, which is subject to technical peer and management review. A data sheet for the selected projects is provided to DOE's Idaho Operations Office (DOE-ID) for concurrence. The continuing and proposed new LDRD project teams are authorized to start work at the onset of the new fiscal year following receipt of DOE-ID's concurrence, and approval by DOE-NE of the annual LDRD Program Plan.

## RESEARCH PROJECT HIGHLIGHTS

### Success Story

Seismic modeling has always been a keen interest for those conducting probabilistic risk assessments for nuclear energy plants. One LDRD project in this area, right, was so successful that it earned direct DOE funding within its first year. The project is developing a modeling method that considers different types of interactions between soil and buildings during a seismic event (project 14-102).



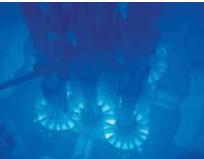
### Societal safety goal

The Nuclear Regulatory Commission's safety goals are conceived as high-level statements on safety philosophy and the role of safety-cost tradeoffs in NRC decisions. The current safety goals address adverse health consequences to individuals from exposure to radiation as a result of accidents. Under current guidelines, nuclear accidents having only minor public health impacts from radiation exposure can cause significant societal disruption (e.g., long-term relocation of a large number of people), and this consequence is not explicitly addressed by existing goals. This LDRD project is studying the formulation of an additional (societal) safety goal to address societal disruption. The team is simulating potential societal disruption from a range of reactor accidents as a first step (project 13-095).

## Advanced reactor component testing

Generation IV nuclear energy technologies are defined by safety, economic, technical and environmental advances. Components relevant to these reactors require performance and integrity evaluation at prototypical conditions. The Advanced Reactor Technology Integral System Test (ARTIST) capability, right, established with this LDRD project provides just such a physical test platform. It is allowing energy systems researchers to advance and integrate emerging technologies such as Advanced Small Modular Reactors, High Temperature Heat Exchangers, Hybrid Energy Systems and Dynamic Grid Energy Storage (project 14-009).



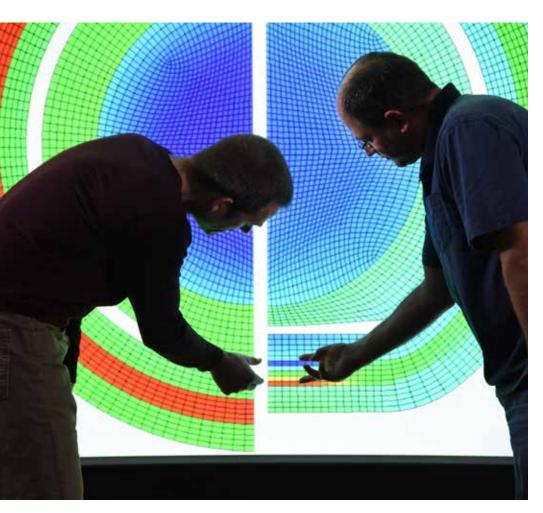


## **Extending reactor life**

A key component in evaluating the ability of light water reactors to operate beyond 60 years is characterizing the degradation of materials exposed to radiation and various water chemistries. Development of advanced in-core instrumentation is critical to DOE's energy security mission to provide world-class facilities for advancing nuclear science and technology. Successful completion of this LDRD project will result in a proven crack growth test rig. Such a testing system could be used by DOE-NE researchers and industry organizations to obtain real-time data about crack growth during irradiation testing in U.S. high flux materials testing reactors (project 13-029).

### Modeling fuel during accidents

Reliably predicting the behavior of nuclear reactor components during abnormal events is essential from both safety and economic standpoints. State-of-the-art computational tools can help. However, empirical models often do not exist for the high temperatures experienced during accidents, and uncoupled simulations are unrealistic during all operating conditions. It is important to replace these approaches with more predictive codes, based on multidimensional, fully coupled multiphysics methods. INL's fuel performance code BISON, below, meets these basic characteristics, offering high potential for the improved computational analysis of fuel rod behavior during accidents. On this LDRD project, novel multiphysics models to describe nuclear fuel rod behavior during accidents were developed, implemented and validated within the BISON code during this fiscal year (project 14-031).



## Safer nuclear fuel

Nuclear engineers have long been interested in fuels with enhanced accident-tolerant characteristics that lengthen the grace period if reactor cooling is lost. Fuel pellets composed of a composite matrix of uranium di-silicide (U<sub>2</sub>Si<sub>2</sub>) and uranium mononitride (UN) are of interest as one such fuel form for light water reactors. Preliminary results of this LDRD project successfully demonstrated the feasibility of producing high-density composites of UN-U<sub>3</sub>Si<sub>2</sub> via the spark plasma sintering process. The U<sub>3</sub>Si<sub>3</sub>-UN fuel conducts heat more efficiently, increases the safety margin of the reactor and may be able to be used in place of fuels in existing light water reactors (project 14-041).

## Irradiation effects in uranium dioxide

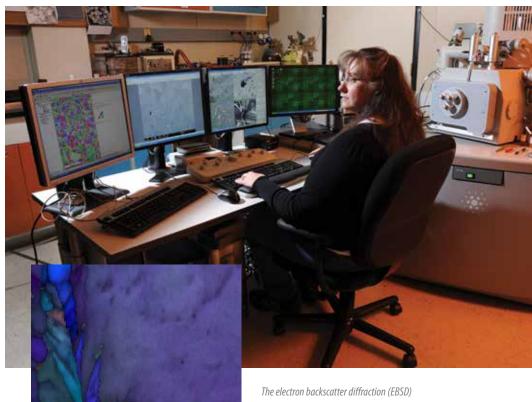
Understanding the impacts of how radiation affects uranium dioxide (UO<sub>2</sub>) at the nanoscale can help engineers better respond to macro-scale material challenges. This LDRD project is simulating the environment inside current and future reactors using ion and proton beams, as well as neutron irradiation via INL's Advanced Test Reactor. The next phase of research will compare and contrast the UO<sub>2</sub> samples exposed to varied environments with actual used fuel samples. The work ultimately supports a more thorough understanding of fuel stability following irradiation and throughout extended fuel storage (project 14-098).

## Nuclear fuel storage integrity

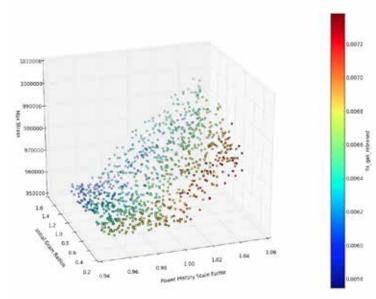
During nuclear reactor operation, an oxidation process within the fuel's protective cladding creates secondary phases called hydrides. Hydrides do not significantly impact the performance of modern reactors, but can lead to embrittlement and cracking during longterm storage. This project is combining modeling with experimental work, right, to predict hydride orientation under dry storage conditions as a function of stress and irradiation history. This question is of great interest to entities including the DOE, the Electrical Power Research Institute, reactor vendors and utilities (project 13-032).

### Nuclear fuel heat transfer

Advanced nuclear reactor fuels will have enhanced safety and performance. Development of such fuels will benefit from a better understanding of how fuel in the nation's current nuclear reactors conducts heat during operation. This LDRD project fabricated pellets of a nuclear fuel surrogate (CeO<sub>2</sub>) to study how heat transfer is impacted by fission gas bubbles and other characteristics at the boundaries between individual crystals of material. The research team determined that a pair of factors dominates resistance to heat transfer depending on specific conditions at these "grain boundaries" (project 13-105).

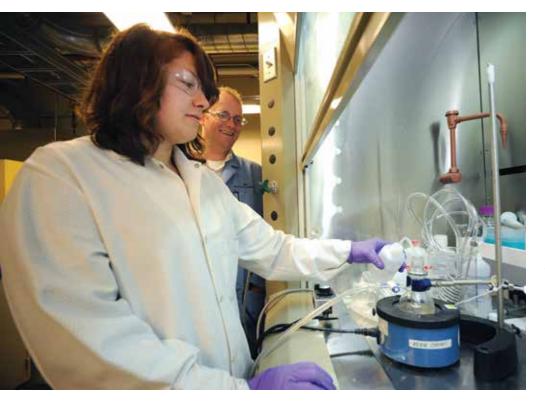


The electron backscatter diffraction (EBSD) technique generated the data for this inverse pole figure (IPF) map, which illustrates the orientation of hydride constituents in nuclear fuel cladding that can lead to embrittlement and cracking during long-term storage.



## Simulation tool validation

High-fidelity simulation tools have benefited many scientific fields and now are being applied to nuclear energy applications. The industry's strong regulatory oversight demands that new tools be validated, and their uncertainties quantified. But uncertainty estimation is a difficult challenge when sophisticated modeling introduces a number of complexities. This project tackles those challenges by finding computational efficiencies that don't compromise predictive accuracy, left. So far, it has successfully coupled the BISON fuel performance code with the RAVEN probabilistic reactor analysis code [project 14-075].



### Nonproliferation accountability

Nuclear nonproliferation efforts rely on specialized detection techniques including mass spectrometry, a process that measures the amount of certain isotopes present in a sample. This LDRD project, left, synthesized a volatile form of neptunium to improve mass spectrometry measurements of nuclear materials and nuclear fuels. Improved, more sensitive measurements will contribute to increased confidence in safeguards accountability and nonproliferation treaty verification (project 14-044).

## Nanotechnology for nuclear fuel recycling

Recycling used nuclear fuel has the potential to separate useful materials from waste products. Traditional separations processes use chemical techniques to collect valuable parts of the used fuel, which has been dissolved in acid. for reuse. This LDRD project builds on the traditional process by combining it with magnetic nanotechnology to simplify the separations process and minimize the waste generated by processing the used fuel. Although it was initially developed for actinide/lanthanide separations, this technology has potential applications in technetium remediation and a wide variety of other critical material separations (project 13-033).

## **Energetic material ignition**

Energetic materials, such as fireworks or materials used for cutting metal, require ignition triggers that must produce a lot of heat quickly. This LDRD project is developing an approach to prevent accidental ignition during a fire or when the material reaches its melting point during storage or transport. These additives aim to enable the energetic mixtures to respond only to specific on-command ignition stimuli while preventing initiation from other stray or unintentional stimuli, below. The project could enhance the safety of personnel in the U.S. departments of Energy, Defense and Homeland Security who routinely use energetic materials for physical security, emergency response and material disposition (project 14-035).

## Success story

A 2012 LDRD project developed an additive to make both energetic materials and ignition triggers less prone to accidental ignition due to static electricity. The patent-pending additive formed the foundation for future LDRD research (projects 12-066, 14-035).





## Success story

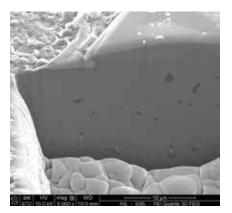
U.S. and international organizations use isotope ratios to ensure nuclear energy facilities *are operating in compliance* with nonproliferation treaty commitments. An LDRD project provided the scientific chemical basis for improved ultratrace isotope ratio measurement that increases accuracy, lowers detection limits and reduces costs. The project yielded scientific publications, an invention disclosure and international university

## Revealing threats within Internet data

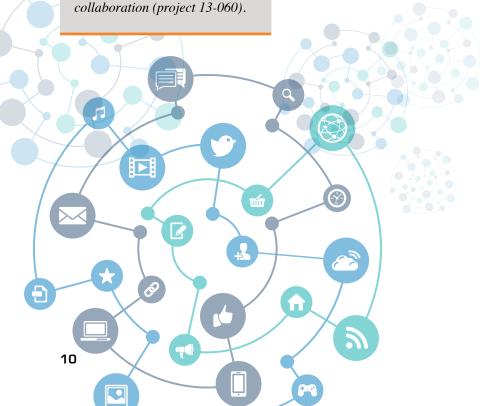
The Internet provides a wealth of freeform, written text (articles, blogs, social media, etc.), known as unstructured data. Transforming information hidden in the unstructured data can improve the nation's ability to prepare for, protect against, respond to and recover from threats to U.S. critical infrastructure. LDRD researchers at INL are working to improve this type of data processing to more effectively reveal potential threats. Researchers have created algorithms that process information from unstructured text. and a framework is in development to logically organize and house the data. The program will perform named entity recognition and geolocation tagging to produce graphical visualizations of data, improving the decision-making processes for critical infrastructure protection (project 14-093).



Advanced armor materials for military and security vehicles must be hard, lightweight and robust. Silicon carbide (SiC) is a candidate material, but it must be encapsulated in a ductile metal structure (which adds considerable weight and volume) or be bonded to a support structure. This LDRD project pursued and evaluated novel methods for bonding ceramic SiC to steel. Specifically, this project evaluated a coating that could enhance the bonding achieved through brazing (a process similar to welding], which melts a second metal to form a bond between two materials (project 14-094).



A focused ion beam created this cross section of coated silicon carbide (SiC) so researchers could examine the interface between the metallic coating (lighter grey) and the SiC (darker grey).



## Passenger vehicle cybersecurity

Modern passenger vehicles include many electronic systems and components including the engine, powertrain, transmission, antilock braking, airbags, power steering, battery and other systems. An LDRD project, right, is exploring remote cybersecurity vulnerabilities, and identifying potential solutions, related to the Controller Area Network Bus (CAN Bus) that influence these systems. The researchers have developed software to decode and spoof network signals and have procured a modern test vehicle. Applications for this work also can address transportation systems related to aerospace, rail and maritime (project 14-032).

### **Evaluating battery materials**

With so many industries interested in improving battery performance, tracking the most effective materials and processing methods is important. INL researchers have begun an LDRD project, right, called "Diagnostics of Advanced Energy Storage Materials" with just that goal in mind. The team will implement various optical, spectroscopic and electrochemical techniques to understand how different manufacturing processes and chemical materials impact the performance of the battery electrodes and battery systems. This year, the team looked at both the formation of the solid electrolyte interphase (SEI) - a specific type of material change that leads to degradation - and how SEI impacts the battery life cycle. They also assessed the performance degradation of siliconbased anodes and the role binders play (project 13-027).





## **RESEARCH PROJECT HIGHLIGHTS**



## **Testing batteries during use**

With their remarkable ability to store power throughout multiple charge and discharge cycles, lithium ion batteries are a popular choice for personal electronics and larger products such as electric vehicles. However, these batteries will eventually degrade with use, and because they are sealed to prevent reactions with air, real-time chemical analysis to improve battery life is not currently possible. LDRD researchers at INL are developing an in-situ measurement process to analyze test battery cells during use. The research began in 2014 with the design and fabrication of a test cell that includes a nanoliter-sized sampling port and a fitting to hold an infrared probe (project 14-095).





#### **Electricity from algae and manure**

The manure from 9 million U.S. dairy cows has the global warming equivalent of 5.8 billion kg of  $CO_2$ . Using the anaerobic digestion (AD) process to treat manure, farms can create a methane-rich biogas to produce electricity or heat. However, the process is expensive and creates nutrient-rich wastewater that is costly to treat. Researchers at the Center for Advanced Energy Studies at INL are working to combine AD with algal biofuel and bioplastic production to address this issue. The algae grow in a photobioreactor, consuming both  $CO_2$  emissions and nutrients from the bioplastic and AD process effluent. The algal biomass also can be used for biofuel production or recycled into the AD. This integrated approach minimizes the environmental impacts of this important industry while producing power and other valuable commodities (project 13-011).

## Chemical manufacturing with microbes

Manufacturing chemicals — especially those developed from petroleum resources — can be an expensive, energy-intensive process. Researchers at INL are turning to bacteria to do some of the hard work. The biological systems of certain extremophiles (bacteria suited for extreme conditions) can be engineered such that their metabolic pathways create desired chemical byproducts. However, this genetic optimization can be achieved on a large scale only with a few types of bacteria. This LDRD project will determine which organisms are best suited to produce specific chemicals. In the first year of the project, researchers successfully created and tested a colorimetric system for identifying genetic modifications, which will be an important step for the rapid screening that will occur as the project progresses (project 13-079).



## Developing micro/smartgrid technologies

The power grid that drives electricity throughout the United States is not optimized for the influx of energy from renewable sources. Researchers at INL are developing an open-source micro/smartgrid control platform and scalable grid simulation models to help understand how to successfully increase the use of renewable resources for both regional and national energy supply. This LDRD project will develop an integrated control system, left, with researchers working closely with industry to begin hardware and software development for future applications. The researchers completed a productive first year, laying out the foundations for the project, getting major pieces of hardware in place and establishing early partnerships (project 14-086).

## AWARDS AND RECOGNITION D RECOGNITION



## MICHAEL TONKS

The computational materials scientist was honored with the 2014 Young Leader Professional Development Award by the Structural Materials Division of The Minerals, Metals and Materials Society. Mike also earned INL's 2014 Laboratory Director's Award for Early Career Exceptional Achievement. He is principal investigator on an LDRD project related to microstructural modeling of nuclear fuel performance (project 13-032).

"I can state, without a doubt, that the MOOSE simulation tool is one of the best, if not the best, to come out of the DOE laboratories in recent years," – Barry Smith, senior computational mathematician at Argonne National Laboratory





## CATHERINE RIDDLE

The nuclear science and technology researcher was honored by the DOE 2014 Innovations in Fuel Cycle Research Awards Program. She won first place in the "Competition for Students Who Attend Universities with less than \$600 Million in 2012 R&D Expenditures." The award was for the LDRD project that supported her doctoral dissertation work (project 11-005).



## MOOSE TEAM

LDRD funding is at the core of INL's Multiphysics Object Oriented Simulation Environment (MOOSE). In 2014, MOOSE became available as open-source software and won a prestigious R&D 100 Award. MOOSE also won the Federal Laboratory Consortium's Far West award for Outstanding Commercialization Success (projects 13-097, 11-061, 10-017).

MOOSE team members (from left) John W. Peterson, Jason Miller, Cody Permann, Derek Gaston, David Andrš and Andrew Slaughter.

## AWARDS AND RECOGNITION D RECOGNITION



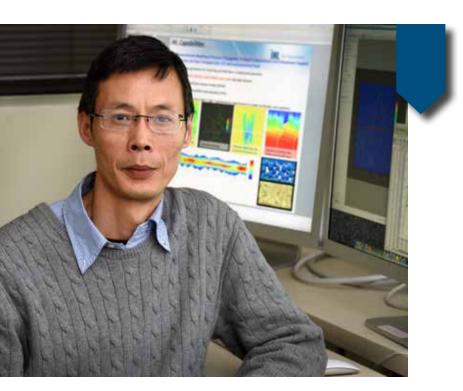
## **PIYUSH SABHARWALL**

The staff scientist received the American Nuclear Society Young Members Excellence Award, which recognizes an early-career nuclear scientist who demonstrates outstanding technical and leadership abilities. Piyush's research focuses on developing new technology for very high-temperature nuclear reactors (projects 12-045, 13-107).

"Piyush has a solid background in nuclear engineering and has actively developed a reputation of excellence with experts throughout the world." – INL scientist Michael G. McKellar



## INL LDRD SNAPSHOT ANNUAL REPORT FY 2014



## HAI HUANG

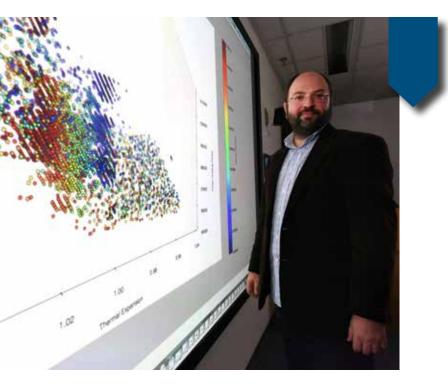
The lead subsurface computational scientist develops models to better understand the physics of fractures and fluids in tight rock formations. His team's models have gained significant interest from the oil and gas industry and resulted in growing funding opportunities from both DOE programs and industry (project 12-113).



## ICIS TEAM

Transforming industrial control systems to be threatresilient is the goal of INL's Instrumentation, Controls and Intelligent Systems (ICIS) Distinctive Signature, a multidisciplinary team of researchers that thrives on a focused research strategy of LDRD projects. In 2014, the ICIS team at INL received an IEEE Region 6 Director's Special Award "For Leadership in the Development and Advancement of Research in the New Field of Resilient, Cyber-Physical Systems" (project 14-103).

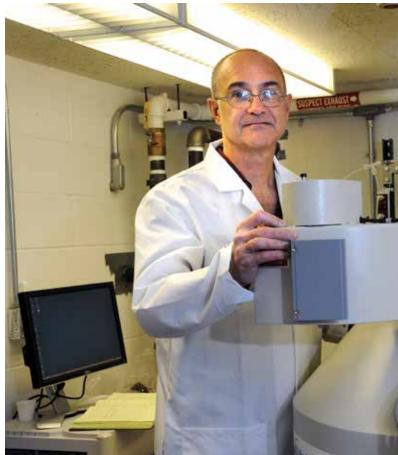
## AWARDS AND RECOGNITION D RECOGNITION



## **CRISTIAN RABITI**

The LDRD researcher was selected as one of two recipients of INL's Science & Technology Deputy Laboratory Director Human Capital Awards. The award honors "those who go the extra mile in supporting interns, undergraduate and graduate student development, and postdoctoral training ... to help recruit the best" (project 14-075).

"It is clear that Cristian is dedicated to enhancing the educational experiences of, and strengthening the INL's nuclear reputation with, top-caliber potential recruits." – INL Thermal Science & Safety Analysis manager Carl Stoots





## LEIGH MARTIN

The radiochemist was one of 10 people named by the Idaho Falls Chamber of Commerce in 2014 as "Distinguished Under 40" for being a dynamic, groundbreaking investigator and mentor. He also was selected as one of two recipients of INL's Science & Technology Deputy Laboratory Director Human Capital Awards (projects 14-044, 13-033).

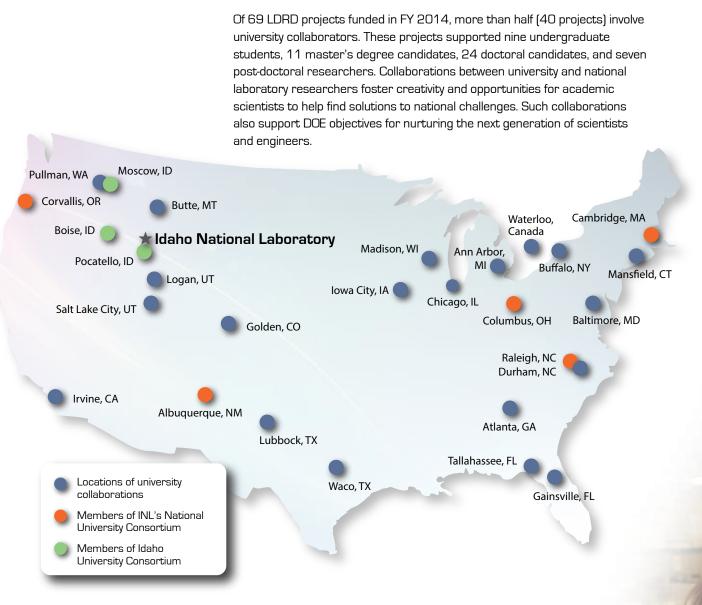


## **BRUCE MINCHER**

The INL Nuclear Science & Technology Fellow was one of three people selected to receive an Idaho Academy of Science achievement award for 2014. Bruce earned the Distinguished Scientist/Engineer award as an expert in actinide solvent extraction, radiochemical separations, radionuclide behavior in the environment and radiation chemistry of organic compounds (project 11-006).

## UNIVERSITY COLLABORATIONS

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## SUPPORTING INL DOCTORAL RESEARCH

Derek Gaston's doctoral research is supported by the LDRD project "Development of a Multiphysics Algorithm for Analyzing the Integrity of Nuclear Reactor Containment Vessels Subjected to Extreme Thermal and Overpressure Loading Conditions" (project 14-104).

The LDRD project "Multivariate Calibration of Complex Simulation Codes using Disparate Types of Evidence" is supporting the doctoral research of **Doug Burns** (project 14-038). **Justin Coleman's** LDRD project "Advanced Seismic Probabilistic Risk Assessment" is supporting his doctoral research. His project is highlighted on page 4 (project 14-102).

The LDRD project "Use of Linear Variable Differential Transformer (LVDT)-Based Methods to Detect Real-Time Geometry Changes during Irradiation Testing" is supporting the doctoral research of **Kurt Davis** (project 14-010).

**Ryan Hruska's** LDRD project "All Hazards Critical Infrastructure Knowledge Framework" is supporting his doctoral research. It is described in the "Revealing threats within Internet data" highlight on page 10 (project 14-093).

The LDRD project "Grid-centric Demonstration of Resilience Technologies" supported **Todd Vollmer's** doctoral research (project 14-103).

## INTERNS AND POST-DOCTORAL FELLOWS

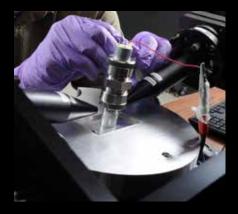
#### **Postdoctoral fellows:**

Wenbo Du Colt Heathman Aaron Johnson Joshua McNally Subhashish Meher Manish Mohanpurkar Sebastian Schunert Bradley Wahlen Yidong Xia

#### Interns:

Jacob Bair Neilsen Beneby William Binder Aaron Butterfield Sayonsom Chanda Alexander Douglass Mara Grinder Shaleena Jaison Mayank Panwar Megan Petti **Michael Picker** Davide Pizzocri Oliver Reed Jaron Senecal Bernard Udu Venkates Venkataramanan Michael West Zexuan Xu Huijin Zhang Jing Zhou

The Laboratory Directed Research and Development (LDRD) program at Idaho National Laboratory advances cutting-edge research and helps develop strategic capabilities that span the lab's nuclear energy, national security and energy security mission areas.









## WWW.INL.GOV/LDRDINL

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