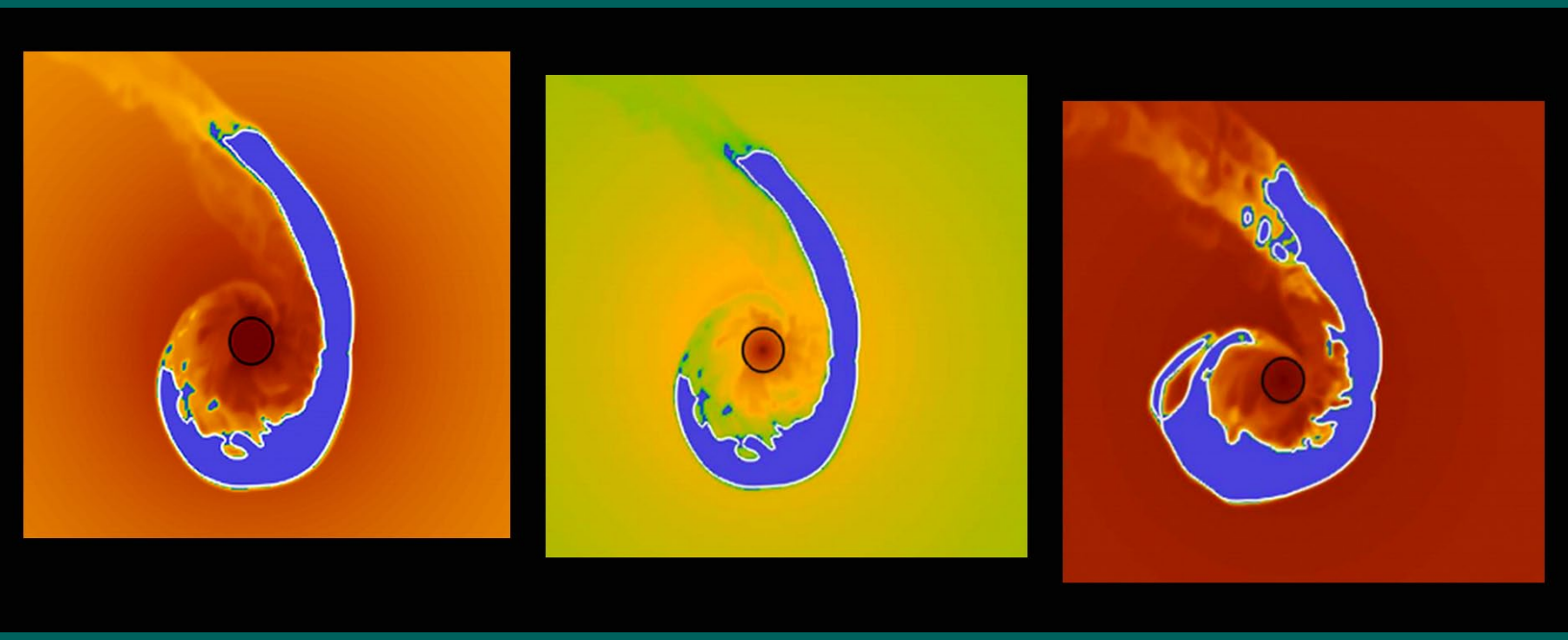
Science and Technology UPDATE

August–October 2012



A bulletin of achievements
at Lawrence Livermore National Laboratory

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TWO YOUNG SCIENTISTS WIN PECASE

Computational scientist Jeffery Banks and design physicist Heather Whitley have been awarded the Presidential Early Career Award for Scientists and Engineers (PECASE), which is the highest honor

bestowed by the U.S. government on outstanding scientists and engineers early in their independent research careers. Awardees are recognized for their efforts in a variety of fields—from advances in power electronics for the electric grid to innovations in scientific computation to new physics developments. DOE nominated the awardees, whose work is funded by a wide range of program offices.

Jeff was nominated by NNSA's Office of Defense Programs for his pioneering contributions in numerical approximations to hyperbolic partial differential equations, and for service in high schools and the scientific community. Jeff received his Ph.D. in applied mathematics from Rensselaer Polytechnic Institute in May of 2006 and has been an employee of LLNL since February 2008, first as a postdoctorial fellow and now as a member of the technical staff.

Heather was chosen for her work using path-integral Monte Carlo techniques to produce accurate quantum statistical potentials for molecular dynamic codes, for applying these methods to first-principles understanding of thermal conductivity in ignition capsules for NIF, and for service to the LLNL Postdoctoral Association. She received a Ph.D. from UC Berkeley in theoretical chemistry in 2007, after being awarded a National Defense Science and Engineering Graduate fellowship.

Heather was involved in the LDRD strategic initiative "The Microphysics of Burning, Hot Dense Radiative Plasmas." The **paper** she published with the principal investigator of that project, Frank Graziani, was a backbone of the work for her nomination. Jeffrey also received LDRD support at critical stages in his award-winning research. Both are shown receiving their plaques from Deputy Secretary of Energy Daniel Poneman.

About the Cover

Simulations at LLNL predict the slow "death by black hole" of a gas cloud at the center of our Milky Way galaxy. "See Galactic cloud's 'death by black hole' predicted," on page 15.

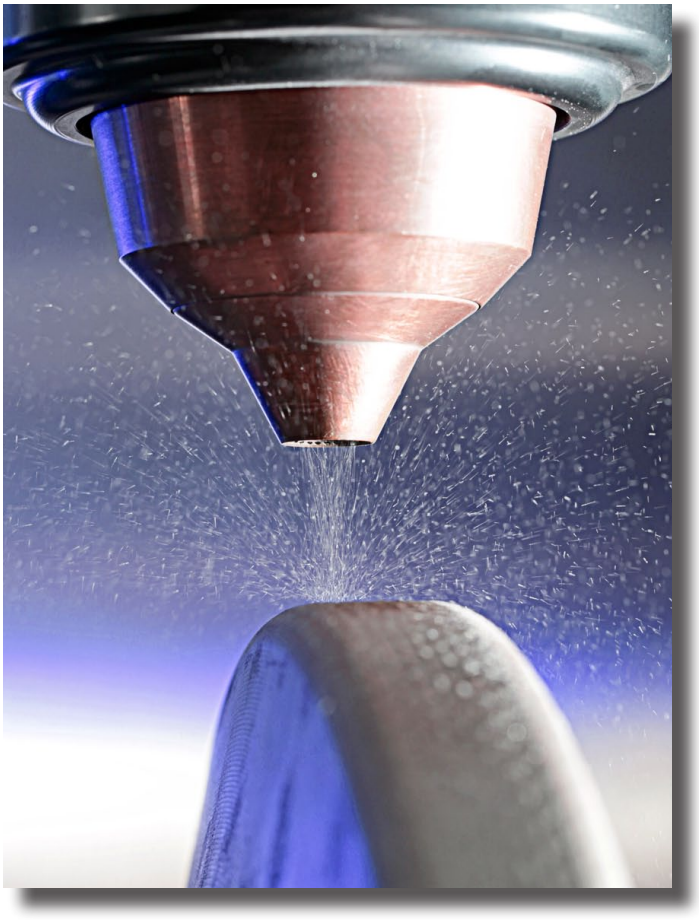
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-7NA27344.

COMPUTATION MANAGER WINS INAUGURAL NNSA S&T AWARD

Michel McCoy, whose pioneering work in high-performance computing (HPC) helped establish Lawrence Livermore as a world-renowned supercomputing center, was **honored** in July with NNSA's Science and Technology Award—the first presented under the newly established award. Michel was recognized for "16 years of dedicated and relentless pursuit of excellence" by NNSA Administrator Thomas D'Agostino, who called HPC "the lifeblood of NNSA science and technology" and said Michel's leadership in HPC "has had a global impact." Administrator D'Agostino added: "Mike McCoy is an example of the difference one individual can make on a team. You have to have a leader who knows how to pull things together and to make tough decisions. That leader is Mike McCoy. If it wasn't for Mike, this would be a very different place." In the photo are, left to right, NNSA Deputy Administrator for Defense Programs Don Cook, NNSA Deputy Administrator for Science and Technology Dimitri Kusnezov, LLNL Director Parney Albright, Mike, Administrator D'Agostino, and WCI Principal Associate Director Bruce Goodwin.

LAB WINS SIXTH R&D 100 AWARD

In addition to the five R&D 100 Awards announced previously, the Laboratory won an additional R&D 100 award this year. The sixth award is for NanoSHIELD, a new coating material developed by Oak Ridge National Laboratory, LLNL, Carpenter Technology Corp., and the Colorado School of Mines. The Livermore work on the award was performed by Frank Wong, a PLS nuclear engineer matrixed to Global Security. NanoSHIELD extends by 20% the life of costly tool steel components used in high-wear applications, such as tunnel boring, construction, drilling, industrial rock crushing, and earth excavation. This year's latest award brings the Lab's total to 143 since it began competing in 1978. In the photo, glassy alloy powder is delivered onto a metal substrate that is then fused to the substrate with lasers to form a NanoSHIELD coating.



RESEARCHER WINS ANS AWARD, IS PICKED TO GIVE LIFE TALK

Nuclear engineer Susana Reyes is the 2012 recipient of the American Nuclear Society (ANS) Mary Jane Oestmann Professional Women's Achievement Award. Susana, who is also vice-chair of the ANS Fusion Energy Division, was recognized for her "leadership in developing detailed hazard and safety analyses for both inertial and magnetic fusion facilities, including NIF and ITER, and future power reactors." The award is given annually for outstanding personal dedication and technical achievement by a woman in the fields of nuclear science, engineering, research, or education. Susana will also give a **presentation** on LIFE at a meeting of the ANS Northern California Section on November 7.

TEAM SHARES AWARD FOR PLASMA PHYSICS RESEARCH

Laurent Divol, Pierre Michel, Debbie Callahan, Ed Williams, Nathan Meezan, and Bob Kirkwood, as well as George Kyrala of Los Alamos National Lab, have been named recipients of the 2012 American Physical Society (APS) John Dawson Award for Excellence in Plasma Physics Research. The award recognizes the team's work on understanding laser–plasma interactions, which led to the successful use of power transfer between crossing laser beams in the NIF hohlraum. This technique has led to the use of two different laser wavelengths to improve the implosion symmetry in NIF ignition targets. The Dawson Award will officially be bestowed at the upcoming APS Division of Plasma Physics annual meeting.

TEAMS WIN NNSA AWARDS OF EXCELLENCE

Four LLNL teams and one individual were honored during the presentation of the NNSA Defense Programs Awards of Excellence in September. The awards were presented at LLNL by NNSA Deputy Administrator for Defense Programs Don Cook. **Peter Anninos** was recognized for his work in resolving two longstanding weapon output problems important to both NNSA and the Department of Defense; the **JASPER Return to Program Team** for successfully resuming high-precision dynamic experiments on plutonium; the **Modern Stockpile Stewardship Techniques Team** for demonstrating stewardship codes and modern assessment methods to identify and assess a potential concern in the stockpile; the **Team for Improvements in Simulation of Physics and Geometric Fidelity** for developing, implementing, and demonstrating on real applications an ASC simulation capability that significantly improves both the physics and the geometric fidelity used for weapon system assessments; and the **9731S Multi-Disciplinary Team** (in the photo below) for successfully executing the first-ever IHE velocimetry pin shot.

POSTDOC WINS IN ENERGETIC MATERIALS POSTER SESSION

George Levesque (left in the photo), a postdoctoral researcher in PLS, won second place in the poster session of the 43rd Annual Fraunhofer Institute for Chemical Technology (ICT) Conference on Energetic Materials, held in Karlsruhe, Germany, June 26–29. George's poster focused on pore size criticality from mesoscale ignition models and was co-authored with PLS colleagues Peter Vitello, Mike Howard, and Larry Fried. The ICT **conference** is an international forum for reviewing the state of the art of new energetic materials, providing a platform for new ideas, and stimulating scientific discussion.

TWO BIOMEDICAL SCIENTISTS NAMED FELLOWS

Carolyn Hall, a microbiologist and analyst with the Biodefense Knowledge Center (BKC), has been selected as a 2012–13 fellow of the Emerging Leaders in Biosecurity Initiative, a competitive **program** at the Center for Biosecurity at the University of Pittsburgh Medical Center designed to create and sustain a multidisciplinary and intergenerational biosecurity community. Carolyn says, "I was very excited to be picked for the program. I'm new to the biosecurity field, and this provides me with a great opportunity to meet leaders in the field and to network."

Dina Weilhammer, a postdoc and immunologist, has been named a 2012–13 American Association of Immunologists (AAI) Public Policy Fellow. Dina is part of a team developing a therapeutic that would activate a person's immune system to provide protection against a variety of bacterial and viral pathogens. "I was very pleased to have been selected as a fellow," said Dina. "I've always believed that scientists need to have more conversations with the general public. It's very important for us to effectively communicate how our work impacts society for its betterment."

NEUTRON IMAGING TEAM RECEIVES DEFENSE PROGRAMS AWARD

PLS researchers David Fittinghoff and Owen Drury and Engineering's Dan Bower, Pat Roberson, Brian Felker, and John Dzenitis will share a 2011 Defense Programs Award of Excellence with their colleagues at LANL and Nevada National Security Site for their work on NIF's Neutron Imaging System. The system produces a two-dimensional image of the source distribution of neutrons from imploding inertial confinement fusion capsules. Such images, which show where fusion neutrons are produced and scattered within the highly compressed fuel assembly, provide critical information on the efficiency of the implosion.

LAB WINS THREE FLC TECH TRANSFER AWARDS

LLNL has once gain been honored for its efforts to commercialize its technologies. The Federal Laboratory Consortium for Technology Transfer, a national network of federal laboratories that develops strategies and opportunities for connecting the labs to the marketplace, has presented LLNL with three awards for excellence in technology transfer in the Far West Region.

An Outstanding Partnership Award went to the **IntelliProbe** optical breast cancer diagnostic system, developed by LLNL, BioTelligent, Inc., and the Russian Federal Nuclear Center to eliminate or substantially reduce the need for biopsies and shorten the time for patients to obtain test results.

An Outstanding Commercialization Success Award went to the **Dynamic Transmission Electron Microscope**, developed by LLNL and Integrated Dynamic Electron Solutions, which provides never-before-seen details of material processes in 15-nanosecond single-shot exposures, allowing scientists to observe what happens at the micro- and nanostructural level when materials are subjected to extreme temperatures, high pressures, and reactive chemicals.

An Outstanding Partnership Award recognizes the **i-GATE Innovation Hub**, a regional public–private **partnership** designed to support small businesses and bolster green transportation and clean-energy efforts by linking national laboratories to entrepreneurs, industry, venture capital, and universities. The hub was created by LLNL, Sandia, and the City of Livermore.

BIODEFENSE KNOWLEDGE CENTER AWARDED BY CUSTOMS AND BORDER PROTECTION

LLNL's Biodefense Knowledge Center (**BKC**) has received an award and plaudits from U.S. Customs and Border Protection for working in a close partnership with the agency over the past 3 years to strengthen its ability to intercept suspicious biological material and equipment. "The work of the BKC has been nothing short of astounding," wrote Thomas Winkowski, assistant commissioner for the CBP's Office of Field Operations, in a commendation letter. Said BKC Director Tom Bates, "This partnership leverages the strengths of the Laboratory and maximizes our impact in fighting bioterrorism." In the photo are Tara O'Toole, DHS Undersecretary for Science and Technology; Dave Shepherd, the DHS project manager for BKC; BKC staff Matt Dombroski, Brent Segelke, and Kristi Swope; and Michael Oraze, Customs and Border Protection Director of Ag/Bio-Terror Countermeasures.

RETURNING SUMMER INTERN RECOGNIZED BY ANS

Crystal Green, a summer intern in LLNL's Nuclear Criticality Safety Division, has been awarded a $1,500 scholarship by the American Nuclear Society's Columbia, S.C. chapter. Crystal is working on a bachelor's degree in nuclear engineering at South Carolina State University. This was her second summer working as an intern at LLNL. Last summer, Crystal, who is originally from Augusta, Georgia, focused on using the LLNL-developed Monte Carlo multitransport code COG to model the French reactor SILENE—work which helped her become one of the first place winners at the student poster symposium. This year, Crysal performed various criticality calculations using COG for the Lab's new Inherently Safe Subcritical Assembly. "The Lab environment is very pleasant," she says. Crystal notes that her most valuable life lessons have come from research. "Sometimes things don't work out the way initially envisioned, but you have to keep a positive attitude to work through the difficulties."

IEEE SENIOR MEMBER NAMED

Hema Chandrasekaran has been named a senior member of the Institute of Electrical and Electronics Engineers (IEEE)—an honor that fewer than 8 percent of IEEE members attain and which recognizes significant contributions, achievements, publications, course development, and technical direction in IEEE-designated fields. Hema has done extensive work with NIF's velocity interferometer for any reflector (VISAR), including the design and implementation of a shot data analysis module. IEEE is the world's largest professional association dedicated to advancing technological innovation and excellence.

PHYSICIST EXPLAINS LLNL OPTICS ON PBS SHOW

Bill Craig, who led the Laboratory's x-ray optics design and testing work for NASA's **NuSTAR** satellite (which **launched** on July 13), appeared in an episode of the PBS multimedia series *Quest* titled "Black Holes: Objects of Attraction." (The entire episode can be **viewed online**.) Bill explains how x-ray optics are able to focus x-rays to obtain images of black holes in unprecedented detailed and to visualize and "extreme objects" that have never been directly seen before, such as relativistic jets.

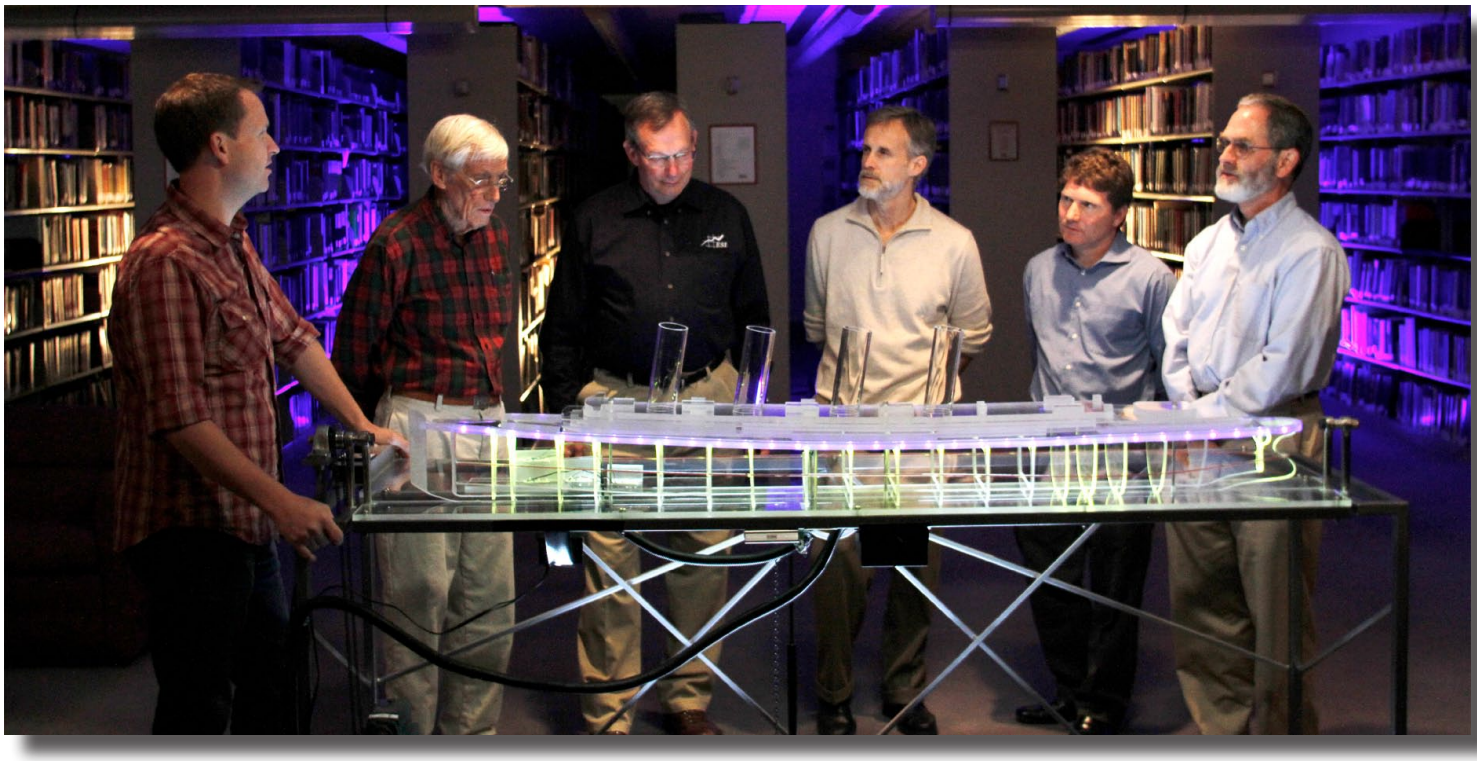
NIF DIAGNOSTICS WORK PRESENTED AT ACS MEETING

Laboratory researchers gave presentations about NIF's diagnostic equipment in a symposium organized by LLNL's Dawn Shaughnessy and LANL colleague Robert Rundberg at the American Chemical Society's Meeting on Materials for Health and Medicine, held August 19–23. Carol Velsco and LLNL colleagues described the Radiochemical Analysis of Gaseous Samples (RAGS) apparatus for NIF nuclear diagnostics.

In addition, Julie Gostic and LLNL colleagues discussed the role of solid debris collection in a variety of inertial confinement fusion experiments at NIF, while Darren Bleuel and his colleagues from LLNL, the University of New Mexico, and Sandia described the extensive suite of neutron activation diagnostics used to measure neutron yields at NIF. The radiochemical diagnostics were also summarized in an **article** in *Chemical & Engineering News*.

EXPLOSIVES EXPERTS TAPPED FOR *LUSITANIA* DOCUMENTARY

Filmmakers producing a National Geographic documentary about the sinking of the British passenger ship *Lusitania* by a German submarine during World War I went to a team of experts at LLNL's High Explosives Applications Facility (HEAF) for help solving a nearly 100-year-old mystery: what caused a massive explosion 15 seconds after the initial torpedo strike? Experts at HEAF conducted both computer simulations and actual explosives **testing** to rule out various theories about the second explosion. The photo shows a preliminary meeting at LLNL's library between (left to right) historian Martin Morgan, venture capitalist and *Lusitania* wreck owner Gregg Bemis, marine engineer Ken Smith, and LLNL's Randy Simpson, Lee Glascoe, and Jon Maienschein.



SEQUOIA AMONG YEAR'S MOST WORLD-CHANGING INNOVATIONS

The Livermore–IBM team responsible for Sequoia, a Blue Gene/Q supercomputer that in June was named the world's fastest, have been **designated** among the top 10 world-changing innovators for 2012 by *Popular Mechanics*. The magazine cites Sequoia as an example of DOE's promotion of its supercomputing capabilities "to help U.S. companies do high-speed R&D for complex products" and "to help the country stay competitive in a world where industrial influence matters as much to national security as nukes do."

LAB SECURES SUNSHOT FUNDING

Lab researchers have secured funding from the DOE SunShot **initiative** to supply U.S. industry with national lab expertise in advanced solar photovoltaic technology. The Laboratory's Vince Lordi will lead the new project, which will leverage Livermore's advanced computational tools and sophisticated imaging techniques to advance the state of the art and enable higher efficiency solar cells that meet aggressive new DOE goals and that can be manufactured commercially. The project is a collaboration between LLNL, the University of Illinois, Nanosolar Inc., and the National Center for Electron Microscopy at LBNL. The project's total budget is $900K over 3 years and brings about $600K of new funding to LLNL.

ENGINEER HONORED BY ASME

Ron Hafner, who for the past year has chaired the American Society of Mechanical Engineers (ASME) Pressure Vessels and Piping (PVP) Division, was recently honored by ASME with two awards: the ASME Board of Governors Award, which was presented to Ron as the outgoing PVP Division Chair, and the ASME Dedicated Service Award, which "honors unusual dedicated voluntary service to the Society marked by outstanding performance, demonstrated effective leadership, prolonged and committed service, devotion, enthusiasm and faithfulness." The awards were presented at the 2012 Pressure Vessels and Piping Conference, held July 15–19 in Toronto, Canada.

AWARD FOR BEST INTERACTIVE PRESENTATION

Jonathan Hopkins received the Best Interactive Presentation Award for his presentation at the Compliant Mechanisms Symposium of the American Society of Mechanical Engineers 2012 International Design Engineering Technical Conferences, held August 12–15 in Chicago. Jonathan presented a paper he authored with Kyle Lange and Chris Spadaccini, titled "Synthesizing the microstructure of thermally actuated materials using freedom, actuation, and constraint topologies," which demonstrates how the principles of the freedom, actuation, and constraint topologies synthesis approach may be applied to the design of compliant microstructural architectures that possess extreme or unusual thermal expansion properties.

IN SUPPORT OF TEST BAN TREATY: AWARD-WINNING SEISMIC AND GAS-SAMPLING TESTS

A team of LLNL researchers shared a 2011 Defense Programs Award of Excellence with colleagues at LANL, Sandia, and other organizations for their work on the first two shots of the Source Physics Experiment (SPE), a series of explosive shots at the Nevada National Security Site (NNSS) to collect data for improving models used for arms control and nonproliferation treaty verification. The award was presented to NNSS researcher Catherine Snelson, director of the SPE tests, by NNSA Deputy Administrator Don Cook at NNSS on September 13.

Prior to this award, the SPE team had successfully **conducted** the third SPE test. Announcing the third test, NNSA Deputy Administrator for Defense Nuclear Nonproliferation Anne Harrington said, "These Seismic Source Physics Experiments are significant achievements in the United States' efforts to develop, validate, and improve on emerging technology that will be used to assure compliance with the Comprehensive Nuclear Test Ban Treaty."

Finally, PLS and Engineering personnel helped design, build, and deploy five "smart" gas samplers at the National Center for Nuclear Security Gas Migration Test Bed, located at NNSS, also in support of the Test Ban Treaty. The first injection was conducted in early September to evaluate how subsurface gases can be used as clues in detecting a clandestine underground nuclear test.

RESEARCHERS ORGANIZE, PRESENT AT ADDITIVE MANUFACTURING SYMPOSIUM

Wayne King, along with staff from DOE, the Atlantic Council, the White House's Office of Science and Technology Policy, the National Institute of Standards and Technology, the Institute for Defense Analysis, and Virginia Tech, organized the Additive Manufacturing Symposium—Preparing for National Prominence in a Disruptive Technology, held on August 20 at the White House Conference Center. The purpose of this symposium, sponsored by DOE and LLNL, was to bring together national leaders engaged in the policy, science, and technology of additive manufacturing (AM) to engage policy and research leaders in a dialogue on what potential AM has on the horizon as a disruptive technology, create a working group for dialogue and monitoring of AM research and policy issues, produce a policy report with recommendations on future actions to facilitate national adoption of AM, and to stage toward a larger summit in winter 2013 involving all AM major players nationwide, with select international visitors. Fifty-four participants from 19 federal agencies attended. Also in attendance were WCI Principal Associate Director Bruce Goodwin, who spoke on the national security implications of additive manufacturing; Associate Director for Engineering Monya Lane; and Anantha Krishnan.

LICENSEE RELEASES NEW NUCLEAR DETECTOR

Detective 200 is the latest addition to LLNL licensee ORTEC's Detective family of products, which are said to be the "gold standard" in gamma-ray-emitting radionuclide identifiers, deployed globally to prevent the illicit trafficking of nuclear materials. The Detective 200 is a new breakthrough radiation identification instrument designed to be compact, highly sensitive, and transportable and for a wide array of nuclear security applications, including mobile, maritime, and portable monitoring.

RESEARCHER GIVES KEYNOTE, INVITED TALK

Tarabay Antoun gave an invited talk entitled "Correlation of Observed Macroscopic Response to Underlying Deformation Mechanisms" (co-authored by LLNL colleagues Oleg Vorobiev, Eric Herbold, and Scott Johnson) at the TomoDamage 2012 **meeting**, held on August 29–31. Tarabay also chaired a session on modeling. Attendance at this meeting, which was organized by the U.S. Office of Naval Research Global and hosted by the Fraunhofer Institute for High-Speed Dynamics, was by invitation only. The TomoDamage meetings provide a forum for discussing the state of the art of x-ray, electron and neutron tomography applied to the detection and characterization of damage in various materials, for the purpose of providing data for predictive numerical simulations.

Tarabay also presented a keynote address at the International Workshop on Computational Mechanics of Materials, held in Baltimore, September 24–26. The presentation—titled "Application of mesoscale simulations toward the development of predictive models for deformation and failure of frictional brittle materials" and coauthored by PLS colleagues Eric Herbold, Oleg Vorobiev, and Lee Aarons—was part of a mini-symposium devoted to modeling material damage across varying physical scales.

TECHNOLOGY FOR REMOVING VIDEO DISTORTION LICENSED

The Laboratory executed a limited, nonexclusive patent license with EM Photonics, Inc. to commercialize a technology titled "Speckle Imaging for Video and Images" for the computer software market; specifically, for removing distortion from video images. EM Photonics, a small business in Newark, Delaware, develops high-performance computing and embedded systems solutions primarily for image processing, scientific computing, and linear algebra.

BEST PRESENTATION AWARD AT CHEMICAL CONFERENCE

A presentation by postdoc Kyle Sullivan, describing research on the preparation and characterization of thermite composites, was chosen as the best oral presentation at the 9th International Symposium on Special Topics in Chemical Propulsion, held July 9–13 in Quebec City, Canada. The presentation reported emerging technologies in additive manufacturing to synthesize and investigate the reaction mechanism of thin films of thermites deposited onto fine-featured patterned electrodes.

This work was supported by the LDRD strategic initiative "Disruptive Fabrication Technologies" (11-SI-005). Kyle presented the work on behalf of team members Josh Kuntz and Alex Gash.

GRAVITY TOMOGRAPHY: DTRA FUNDING AND KEYNOTE

A joint project between LLNL and partner company AOSense, Inc. to develop a mobile system that uses cold-atom atomic interferometry to detect hidden masses by their effect on the local gravity gradient has been selected by the Defense Threat Reduction Agency for funding. The project will design, model, build, and test a prototype gravity sensor suitable for field operation. The budget for the three-year project is $3M, with $900K coming to LLNL. AOSense will have overall leadership of the project; Livermore's participation will be led by Steve Libby. Potential applications of the system include nuclear materials detection, treaty verification, emergency response, cargo screening, and detection of subterranean structures. The same cold-atom interferometry technique also has possible application in high-precision measurements of the gravitational constant. The project is an outgrowth of basic research in gravitational physics being investigated in an LDRD project led by Steve.

Steve also gave the keynote talk at this year's Hertz Foundation East Coast Retreat, **held** October 26–28 at Thompson Island, Boston Harbor. In his talk—"Quantum Coherent Cold Atom Interferometers Meet Applications: Inertial Motion Sensors and Gravitational Tomography"—Steve reported results from a current LDRD Labwide project and related projects that are developing gravity gradiometers based on atomic interference effects to address outstanding problems in both national security and the fundamental physics of gravity.

NNSA PRESS RELEASE ON NUCLEAR SECURITY CITES LLNL RESEARCH

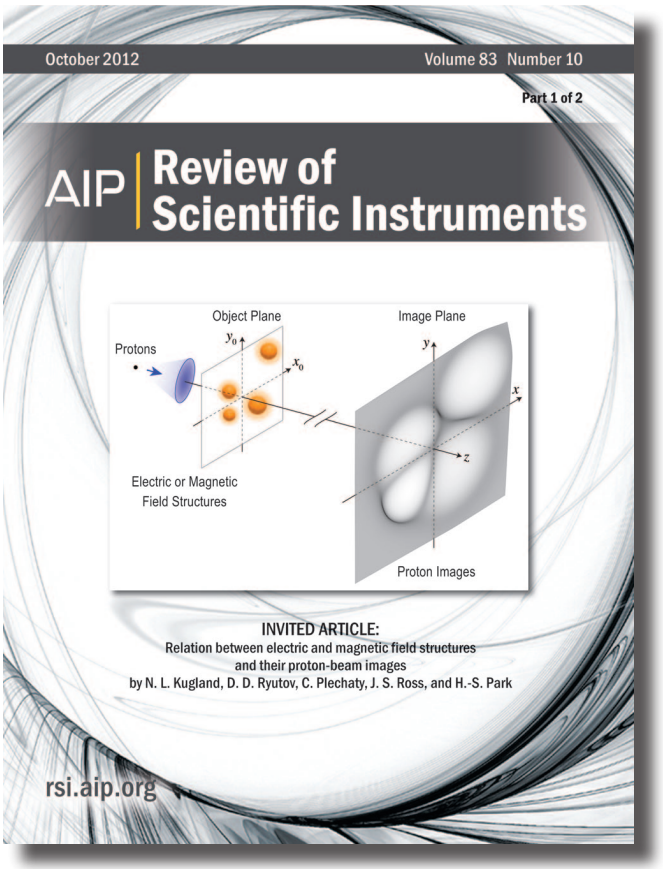
Research conducted by PLS researchers Kim Knight and Amy Englebrecht, in collaboration with four Ukrainian institutes, to identify signatures of different uranium-bearing material samples was **highlighted** in an NNSA press release. Their work aims at enhancing Ukraine's ability to counter illicit nuclear and radiological material trafficking and is sponsored by NNSA's Global Initiatives for Proliferation Prevention, which seek to mitigate the risk of proliferation through collaborations between foreign research institutions and U.S. national laboratories and industry.

FULL CELL LICENSEE WINS INNOVATION AWARD

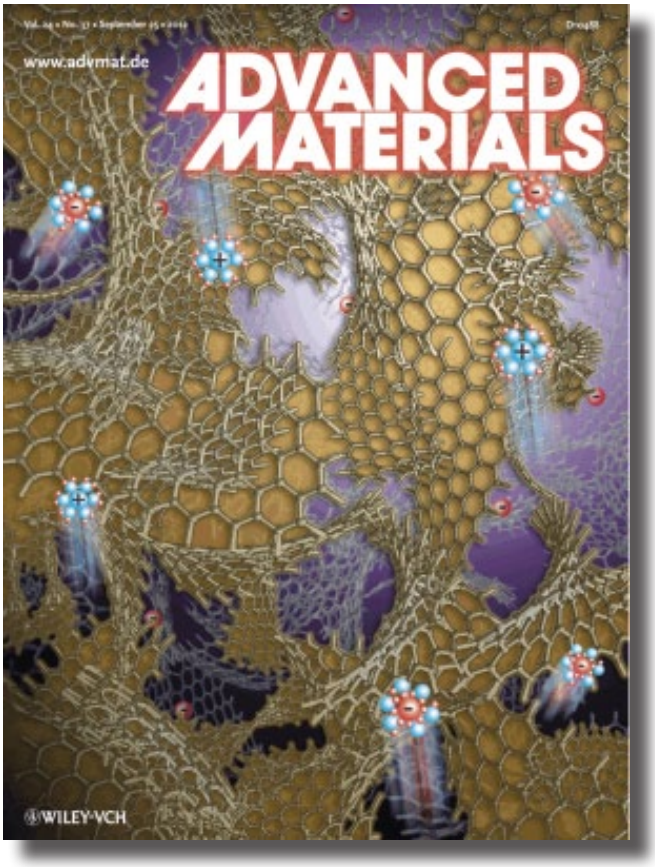
Zinc Air, Inc., which licenses LLNL fuel cell technology, was **honored** with an Innovative Business Award at the First Annual Governor's Innovation Day and Awards Dinner. The Columbia Falls-based company was one of nine Montana firms recognized by Governor Brien Schweitzer as "companies that exemplify the opportunities businesses have in Montana." Zinc Air is using the LLNL-developed safe, sustainable, and cost-effective technology to devise a grid storage system capable of breaking the cost–benefit threshold, which is currently limiting the widespread adoption of fuel cells in this field.

THEORY ON PROTON IMAGING OF PLASMAS ON *RSI* COVER

Point-projection proton imaging is a powerful technique for visualizing the electric and magnetic fields in high-energy-density plasmas. Although this technique has been used for about ten years, there has been no general analytical framework for understanding how proton images are formed by the electric and magnetic fields present in a plasma. Now, in an invited **article** featured on the cover of *Review of Scientific Instruments*, this gap has been filled. LLNL authors Nathan Kugland, Dmitri Ryutov, Chris Plechaty, Steven Ross, and Hye-Sook Park use an approach similar to optical shadowgraphy, but with the electric or magnetic potential serving as a proxy for refractive index. This paper provides the first detailed analysis of proton-image caustic formation and provides a library of proton images from variously shaped fields that can be used to make experimentally obtained proton images more quantifiable. This work will clearly serve as a starting point for any future quantitative analysis of proton images.



NEW MATERIAL WITH "REMOTE CONTROLLABLE" PROPERTIES



Researchers here have developed a new material whose physical properties can be dynamically changed by an external signal. A paper **featured** on the cover of *Advanced Materials* describes a method to fabricate graphene-based bulk materials from polymer-derived carbon foams. "The new technique is inexpensive, scalable, and yields mechanically robust, centimeter-sized monolithic samples that are composed almost entirely of interconnected networks of single-layer graphene nanoplatelets," said Livermore's Ted Baumann, who developed the synthetic approach. Lead author Juergen Biener stated, "This is a potentially game-changing concept in materials science. Just imagine what you could do with a bulk material with properties you can change dynamically by an external variable. For example, you could switch a bulk material dynamically between a conductive and an insulating state." The cover image depicts the material's 3-D structure, consisting of a 3-D network of single-layer graphene nanoplatelets.

CATALYST WORK ON INSIDE COVER OF *CHEMISTRY*

The inside cover of the August 20, 2012 issue of *Chemistry, A European Journal* featured a **paper** by LLNL researchers Stephen Harley and Harris Mason and their UC Davis collaborators on the chemistry of a cobalt-hydroxide water-oxidation catalyst that is an attractive candidate for catalyst-functionalized photo-electrodes that drive direct water oxidation upon exposure to light. Until now, there has been debate about the chemical structure of this material, particularly whether phosphate ions bond directly to cobalt sites, but the findings of Harley et al. support the idea that most phosphate ions are mobile in the interlayer region between the metal–hydroxide layers and interact with nonbonded cobalt(II) arranged in sheets in the material. These findings, which could lead to further optimization of this class of catalysts, were also **highlighted** in the international edition of *Angewandte Chemie*.

NEW DESALINATION TECHNIQUE IS FASTER, MORE ENERGY EFFICIENT

In a **paper** published as a "Hot Article" by *Energy & Environmental Science* and featured on the back cover of the journal's November issue, Livermore researchers describe a new capacitive desalination technique that could reduce the cost and time of desalinating seawater. In capacitive desalination, a voltage is applied between two porous electrodes to adsorb ions onto the electrode surface and thus remove them from the feed stream. Traditionally, due to the small pore sizes of the electrodes, the feed stream flows between the electrodes and through a dielectric porous separator. The new technique, called flow-through electrode capacitive desalination, uses new porous carbon materials with a hierarchical pore structure, allowing salt water to easily flow through the electrodes themselves. Advantages over traditional flow-between system include desalination that is faster and more energy efficient. The image depicts desalination with the new hierarchical porous carbon material, with the feed stream passing directly through the electrodes.

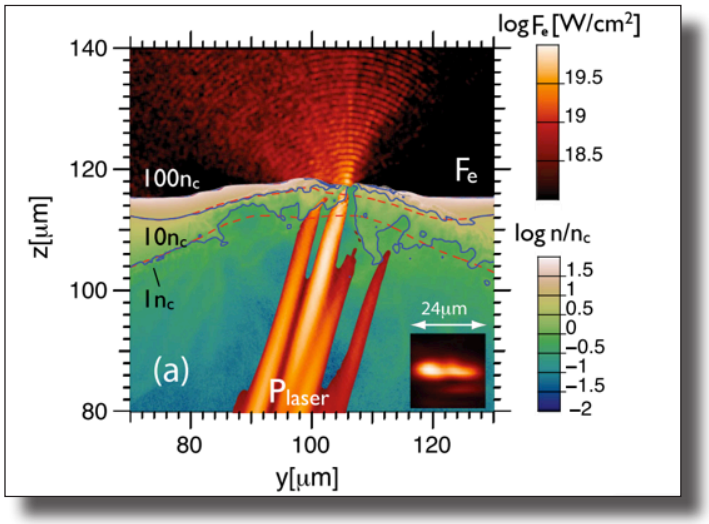
LABORATORY DOMINATES *PHYSICS OF PLASMAS* TOP 10

Four of the five **most-cited papers** for all time in *Physics of Plasmas*, as well as five of the top 10 papers, have LLNL researchers as first authors—a clear signal that the external scientific community recognizes LLNL's signature core competencies in plasma physics and high-energy-density science.

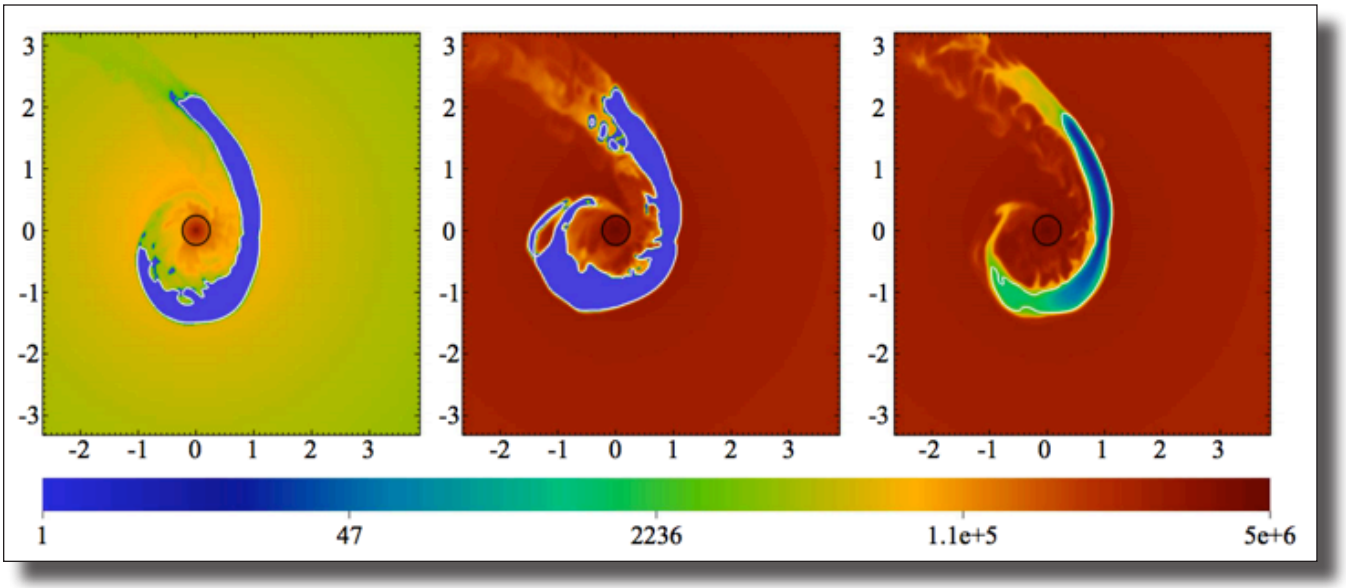
GALACTIC CLOUD'S "DEATH BY BLACK HOLE" PREDICTED

Published in *Astrophysical Journal*, supercomputer simulations prepared by computational physicist Peter Anninos and astrophysicist Stephen Murray-and, along with former Lab postdoc Chris Fragileand (now at the College of Charlestown) and his student, suggest that a black hole may devour much of an approaching cloud of dust and gas known as G2. The black hole, Sgr A*, is in the center of the Milky Way and is 3 to 4 times more massive than our Sun. Using the Cosmos^{++} code developed by Peter and Stephen, the team conducted six **simulations**, all showing that the cloud will not survive the encounter, which will be observable over the next several years. The figure gives pseudocolor plots of the isentropic constant $\varkappa$ for three models' predictions of the cloud's state in May 2013.

PAPER EXPLORES NEW REGIMES IN FAST IGNITION



In *Physical Review Letters*, a team led by Yuan Ping **describes** a diagnostic they created to record critical surface motion during picosecond-scale relativistic laser interaction with a solid target, and explain that a redshift in single-shot measurements that decreases with time corresponds to a slowdown of the boring of a hole into the overdense plasma. Simulations agreeing with the data support a simple explanation of the slowing-down of the critical surface: momentum conservation between ions and reflected laser light. The figure is a snapshot of laser Poynting flux, electron density, and electron energy flux at peak power in the 2-D PIC simulation. The red dashed contour



lines and the blue lines represent t = 0 and t = 2.2 ps, respectively. The inset is a typical on-shot Titan vacuum focus.

"UNCONVENTIONAL" STRATEGIES NEEDED TO PRESERVE OCEANIC SPECIES

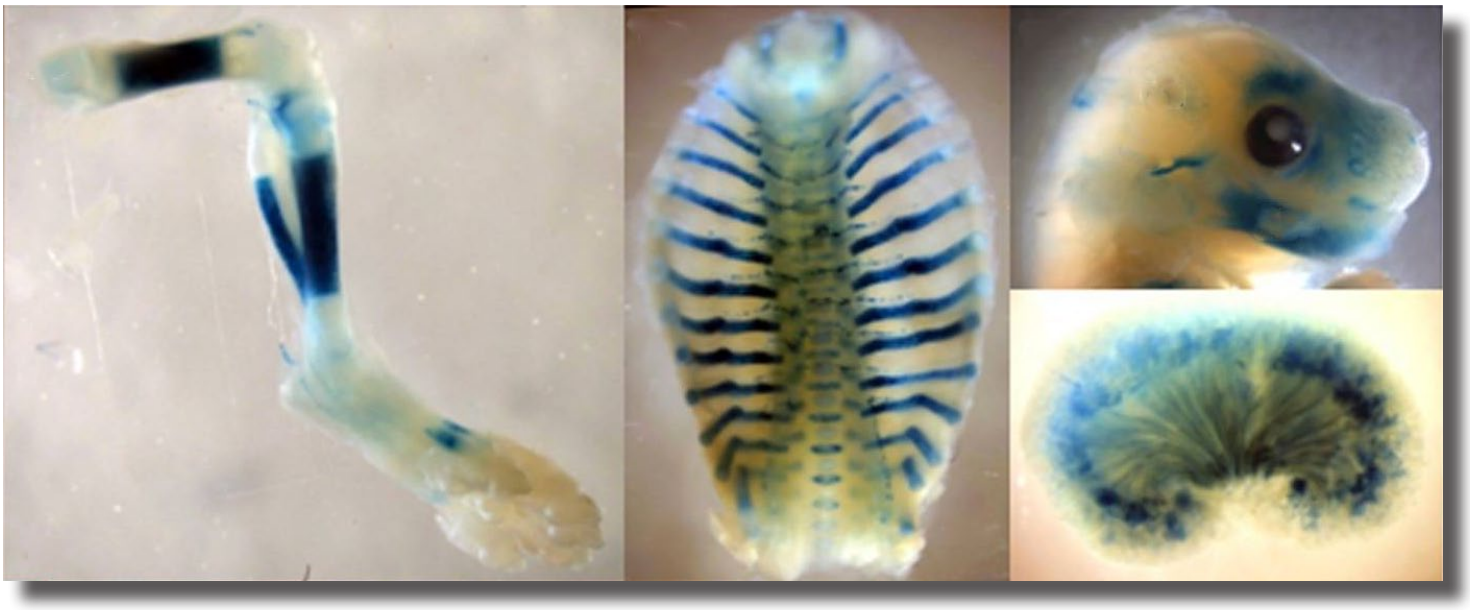
A group led by UC Santa Cruz researcher and LLNL visiting scientist Greg Rau conclude, in a **paper** in *Nature Climate Change*, that many marine species will be harmed or wiped out if levels of carbon dioxide continue to increase, that current protection policies and management practices are unlikely to be enough to save them, and that unconventional, non-passive methods to conserve marine ecosystems need to be considered if various marine species are to survive. Says Greg, "We are concerned that conventional marine environmental management methods may prove to be insufficient or not fully achievable in the time frame necessary to ensure the preservation of current marine ecosystems and their services in the face of CO_2-related threats." Other team members are from The Nature Conservancy in Hawaii and the University of Queensland in Australia.

COLD CASES SOLVED WITH CAMS TECHNOLOGY

In the September 2012 issue of the *Journal of Forensic Sciences*, Bruce Bucholtz of the Center for Accelerator Mass Spectrometry (CAMS) and a team of international collaborators **report** on a multidisciplinary approach for reliably identifying the remains of missing persons in "cold cases" occurring in the last 60 years. By combining an age-dating technique developed at CAMS with recently developed anthropological analysis and forensic DNA techniques, the research team was able to identify the remains of a missing child 41 years after the discovery of the body. This example highlights the enormous potential of combining radiocarbon analysis with anthropological and mitochondrial DNA analyses to identify remains. Bruce's work at CAMS has shown that the increase in carbon-14 caused by above-ground nuclear testing in the 1950s and '60s is recorded in dental enamel, and that teeth can be dated with this "bomb-pulse" radiocarbon to establish the date of birth to within one to two years. The figure shows plant matter found inside a human skull, analysis of which was combined with radiocarbon analysis to narrow down the time and location of the crime.

RESEARCH UNCOVERS MECHANISMS REGULATING BONE FORMATION

Livermore researchers Nicole Collette and Gaby Loots, along with colleagues from UC Davis, UC Berkeley, and Regeneron Pharmaceuticals, have published a **paper** in the online edition of *Proceedings of the National Academy of Sciences* in which they report important discoveries on the mechanisms by which bone formation is regulated. They have identified what appears to be a bone enhancer, ECR5, in the genomic region that is missing in persons suffering from van Buchem disease (characterized by lack of the signaling protein sclerostin), and further identified a protein, Mef2C, that binds to and activates this enhancer. They infer that ECR5 regulates the expression of the SOST gene, and the absence of ECR5 causes van Buchem disease in rodents. Studies of this system are likely to further elucidate additional mechanisms of bone formation and homeostasis. The figure shows the expression, in the neonate skeleton of a transgenic mouse, of beta galactosidase by ECR5.

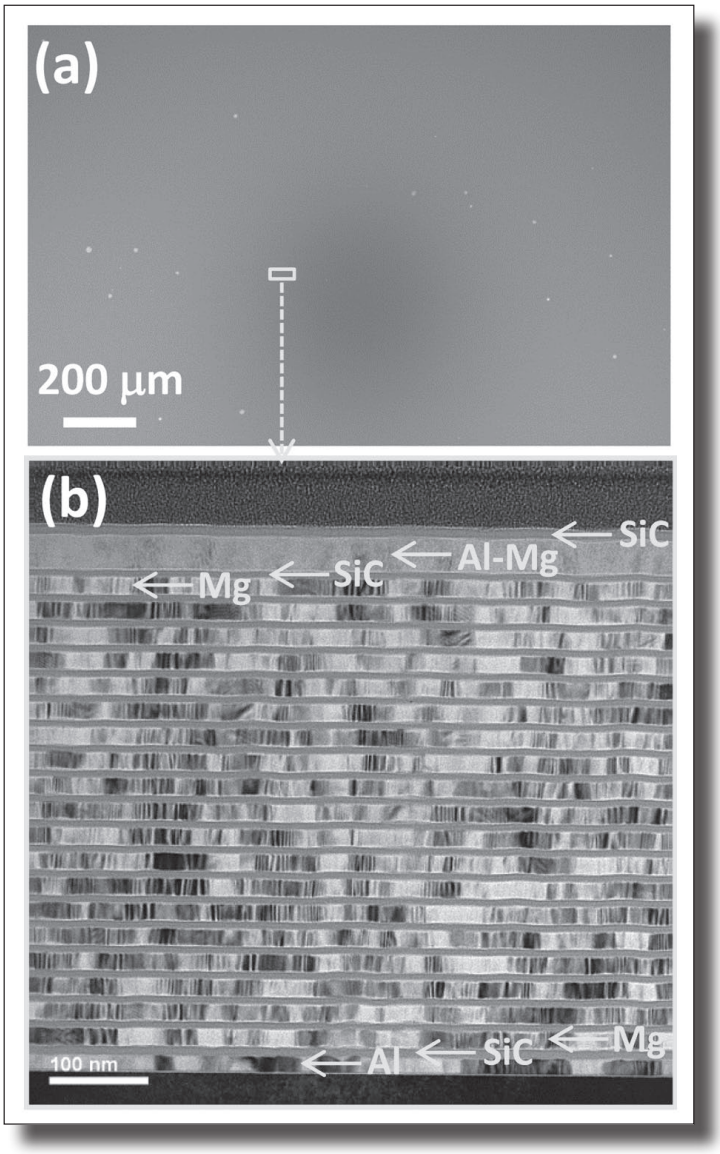


STUDY OF HOT, DENSE MATTER OVERTURNS EXISTING THEORIES

An international collaboration including Livermore's Yuan Ping performed the first-ever controlled studies of extremely hot, dense matter, which, as **described** in *Physical Review Letters*, have overthrown the widely accepted 50-year-old model used to explain how ions influence each other's behavior in a dense plasma. The team used the Linac Coherent Light Source to measure the detailed properties of these states and test a fundamental class of plasma physics for the first time ever, and were able to pinpoint how much energy it takes to knock electrons from highly charged atoms in a dense plasma. "That's a question no one's been able to test properly before," said Oxford University's Orlando Ciricosta, lead author of the study. The research may lead to improved modeling for certain aspects of fusion, as it gives detailed information about the process in which tightly packed atoms begin to lose their autonomy as the orbits of their associated electrons overlap.

TECHNIQUE IMPROVES CORROSION RESISTANCE OF PROMISING OPTICS COATINGS

In a **paper** published in *Applied Physics Letters*, Livermore researchers Regina Soufli, Monica Fernandez-Perea, Sherry Baker, Jeff Robinson, Jennifer Alameda, and Chris Walton explain the origins and mechanisms of corrosion propagation in magnesium–silicon carbide (Mg–SiC) multilayers, whose potential to be the best-performing reflective multilayer coating in the 25–80 nm wavelength region (for applications such as solar observatories and space weather satellites) is hampered by corrosion of the Mg layer. Based on that analysis, they developed and demonstrated an efficient and simple-to-implement corrosion barrier for Mg–SiC multilayers. The barrier consists of nanometer-scale Mg and aluminum (Al) layers that intermix spontaneously to form a partially amorphous Al–Mg layer. The figure gives (a) a scanning electron micrograph of a corrosion-resistant Mg–SiC multilayer film aged for 3 years and (b) a cross-sectional transmission electron microscopy image of a portion of the multilayer, demonstrating a dramatic reduction of corrosion compared to standard Mg–SiC multilayers. This work was supported by LDRD under project 12-ERD-055.



GEOMECHANICS PAPER AMONG TOP 25 DOWNLOADS

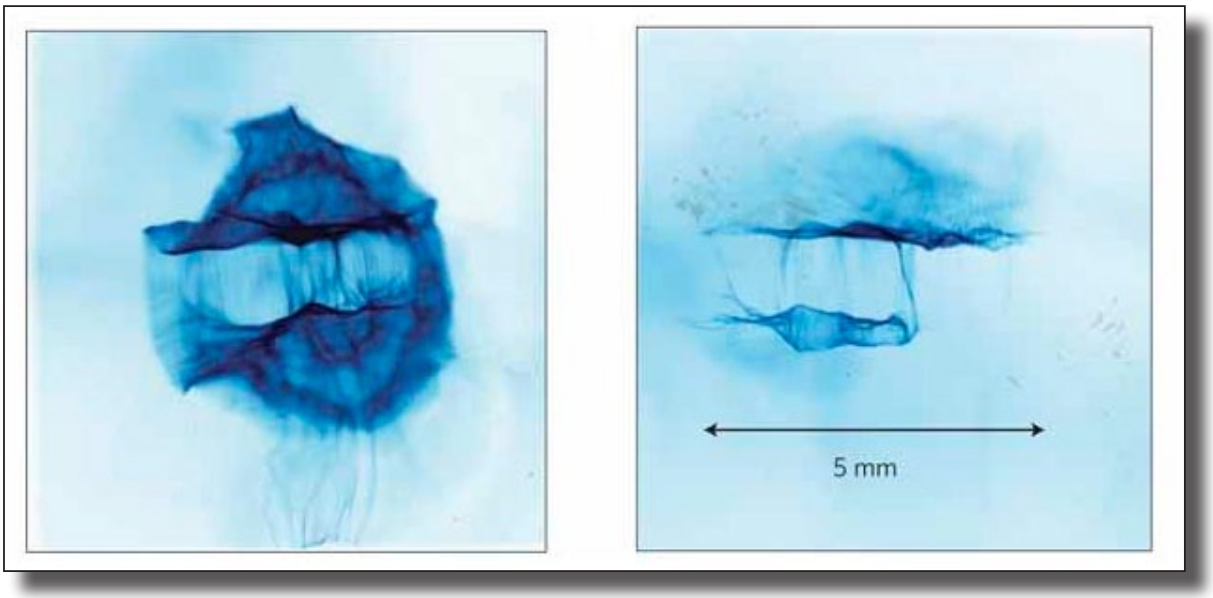
A **paper** by LLNL authors Pengcheng Fu, Scott Johnson, Randy Settgast, and Charles Carrigan has made the list of top 25 **most downloaded papers** over the past 90 days for the journal *Engineering Fracture Mechanics*. Other papers on the list were published between 1998 and 2012. The paper describes a new method for modeling dynamic fracture propagation without requiring high-resolution meshing near fracture tips, and was developed for the Laboratory's work on enhanced geothermal energy systems.

NEW INSIGHTS INTO ACTINIDE ELECTRONIC STRUCTURE

Mark Wall and Patrick Allen contributed to a **study** published in *Proceedings of the National Academy of Science* that significantly advances the understanding of the electronic structure of elements that have electrons occupying f-orbitals. Using a state-of-the-art, synchrotron-based x-ray spectroscopic tool known as resonant x-ray emission spectroscopy, the team measured x-ray spectra for a large number of uranium and plutonium intermetallic compounds, finding "multiconfigurational" electronic structures exhibited by actinide atoms in many of the intermetallic compounds and in pure alpha-phase uranium and plutonium.

BREAKTHROUGH IN SELF-ORGANIZING FIELDS IN PLASMAS

In a breakthrough **announced** in *Nature Physics* and **highlighted** in the journal's "News and Views" section, LLNL researchers have made the surprising discovery of self-organized electromagnetic fields in counter-streaming ionized gases (i.e., plasmas). This discovery relates to an unsolved mystery of science—how highly organized structures can emerge from the random motion of particles. Postdoc Nathan Kugland, lead author of the paper, explains, "We've created a model for exploring how electromagnetic fields help organize ionized gas or plasma in astrophysical settings, such as in the plasma flows that emerge from young stars." This research is being carried out as part of a large international collaboration, Astrophysical Collisionless Shock Experiments with Lasers, led by LLNL, Princeton University, Osaka University and Oxford University, with many other universities participating. Researchers from LLNL conducted the experiments on the Omega EP laser.



The figure gives two frames—4.0 ns (left) and 5.2 ns (right)—of a time sequence of proton images showing the appearance of large-scale caustics in the evolution of self-organized electromagnetic field structures.

NEW APPROACH TO DARK-MATTER SEARCHES WITH EXISTING DATA

A **paper** entitled "First direct detection limits on sub-GeV dark matter from XENON10," co-authored by PLS researcher Peter Sorensen, has been **featured** as an Editor's Suggestion in *Physical Review Letters*. Numerous experiments worldwide are searching for direct evidence of galactic dark matter. The paper describes how existing data from the XENON10 dark matter search experiment can be used to probe for the existence of dark matter particles with masses as low as 10 MeV. This significant advance resulted from looking for electron signals coming not from dark matter–nucleus collisions but from dark matte–electron collisions and are particularly significant because they point the way to future experiments that can probe previously unexplored regions of dark matter parameter space.

METHOD INDEPENDENTLY CONTROLS IONIC AND ELECTRONIC CONDUCTIVITY

Postdoc Cedric Rocha-Leão, working with Vince Lordi, has found a new method to independently control ionic and electronic conductivities in certain solids—a method to control the conductivity of materials that could eventually apply to fuel cells, batteries and gas sensors. The method, **described** in *Physical Review Letters*, uses tailored acceptor-donor co-doping to bind charged native vacancies and selectively modulate ionic but not electronic conductivity, and was developed by using first-principles materials simulations.

FIRST ATOMISTIC SIMULATION OF AZIDE ENERGETIC MATERIAL

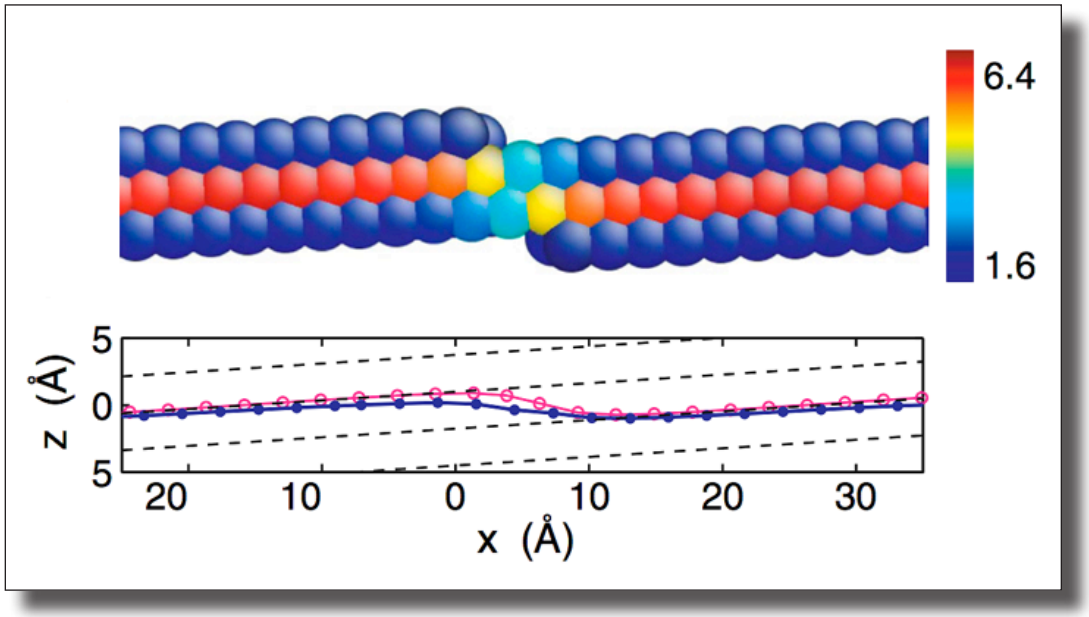
Researchers Riad Manaa, Laurence Fried, and Craig Tarver, in collaboration with former Lawrence fellow Evan Reed (now a professor at Stanford University) and Alejandro Rodriguez (MIT), published a **paper** on ultrafast detonation of hydrazoic acid in *Physical Review Letters*. The manuscript describes the first atomistic simulation of an azide energetic material, HN_3, from the shock front to the completely reacted state and shows that the time scale for complete decomposition is orders of magnitude shorter than that of secondary explosives, approaching the fundamental limiting time scale for chemistry. The team studied several consequences of the short time scale, including a state of vibrational disequilibrium induced by the fast transformations.

ASSESSING RELATIONSHIP BETWEEN AIR QUALITY AND CLIMATE

Climate scientists Daniel Bergmann and Philip Cameron-Smith coauthored a **paper** in *Chemical Society Reviews* that examines the relationship between pollution and climate change. The work focuses on the interactions between methane, ozone precursors, aerosols, and radiative forcing and also assesses the implications for continental-scale air quality of a set of possible 21st century emission trajectories being used as input to the latest round of climate model comparisons. The study concludes that climate change and air-quality processes are interrelated, that confidence in air quality projections is limited by the uncertainty in anthropogenic emission trajectories and in model responses, and that methane, in addition to being a greenhouse gas, degrades air-quality, so controlling methane emissions has dual benefits.

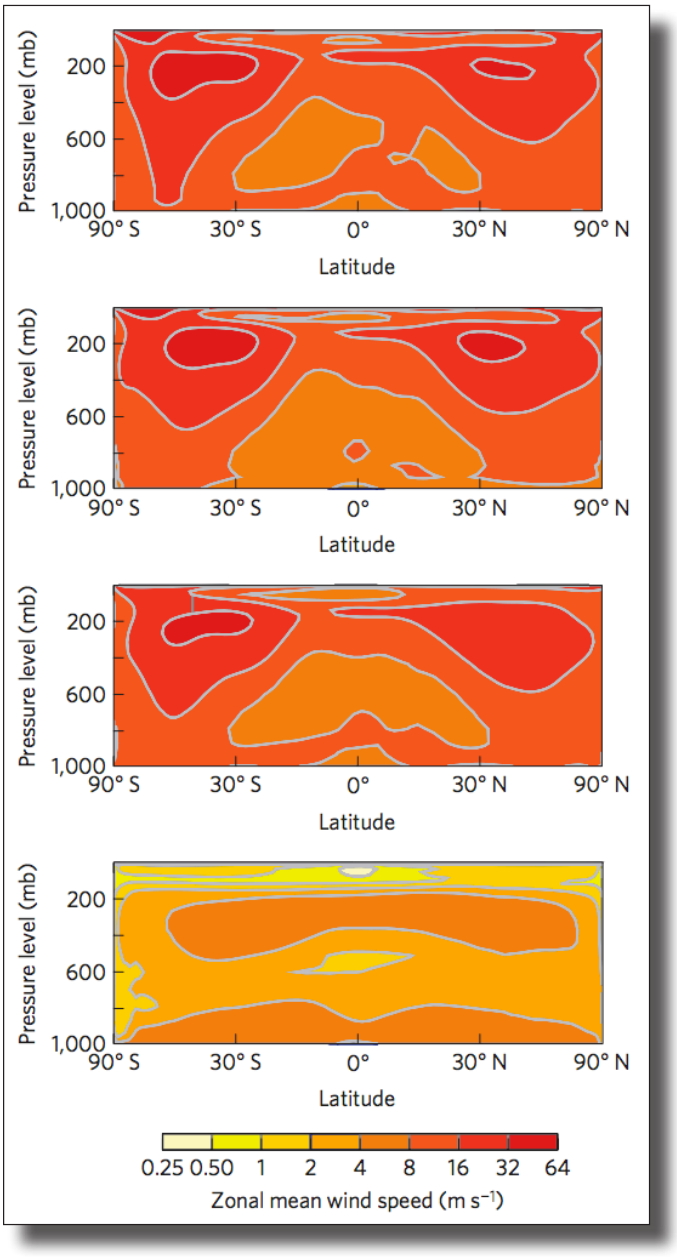
RELATIONSHIP BETWEEN CRYSTAL DEFECTS AND STRESS RESISTANCE FURTHER ELUCIDATED

A paper **published** by Vasily Bulatov, LANL colleague Keonwook Kang, and former Lawrence fellow Wei Cai (now at Stanford University) in *Proceedings of the National Academy of Science* reports on atomistic calculations that carefully examined variations in Peierls stress—an important measure of dislocation mobility—over a range of dislocation orientations in the body-centered-cubic metal tantalum. The calculated variations in Peierls stress as a function of orientation are striking and cannot be fully explained within existing theory, but the team shows that an extension of the standard theory can provide a semiquantitative description of the variations. Their findings also explain why bcc metals are softer at low temperatures than was previously predicted by theory. The figure shows (top) atoms in the core of a dislocation colored according to centro-symmetry deviation and (bottom) model predictions of the equilibrium line shape of the same dislocation.



HARVESTING HIGH-ALTITUDE WIND ENERGY WILL NOT AFFECT GLOBAL CLIMATE: STUDY

In a **study** published in *Nature Climate Change*, postdoc Kate Marvel and colleagues from the Carnegie Institution show that Earth's winds contain enough power to be a primary source of near-zero-emission electric power for the world and that large-scale high-altitude wind power generation is unlikely to substantially affect climate. Kate and team used a climate model to estimate the amount of power that could be extracted from both surface and high-altitude winds, considering only geophysical limits, and conclude that the latter could yield kinetic energy at a rate 4.5 times faster than could wind turbines on Earth's surface—1,800 TW compared to 400 TW. Because present global primary power demand is, in comparison, 18 TW, uniformly distributed wind turbines would be unlikely to substantially affect the Earth's climate, they conclude. The figure shows the zonal mean wind speeds for the cases studied.



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Questions? Comments?

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