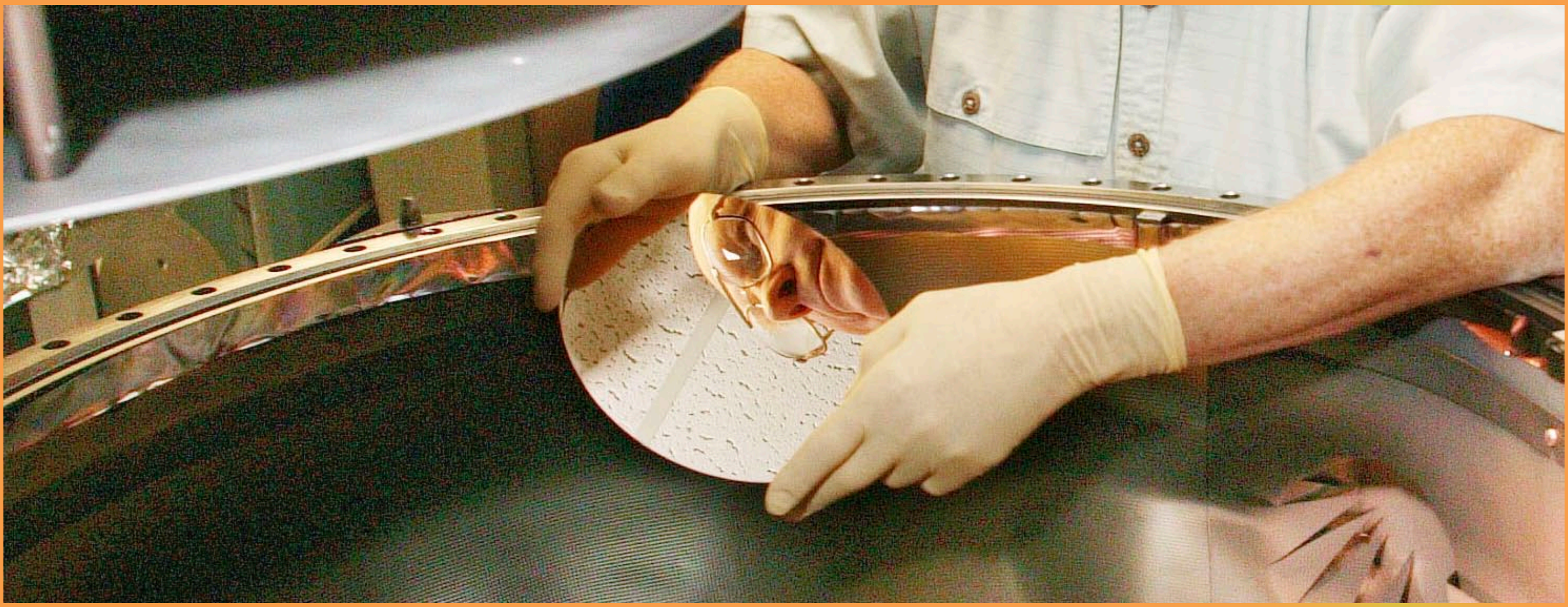
# Science and Technology UPDATE

February/March 2012



A bulletin of achievements
at Lawrence Livermore National Laboratory

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## PAIR OF DEFENSE PROGRAMS AWARDS WON

In the first week of April, seven teams of LLNL researchers were presented with NNSA Defense Programs Awards of Excellence by Deputy Administrator for Defense Programs Don Cook. "There's just no question," he said, "that if we want to look after the safety and security and the reliability of America's nuclear deterrent, we need to put it in the hands of the smartest people who will really ensure that these weapons remain safe, secure, and reliable."

Recognized were the Energy Balance Assessment and Application Team (shown in the photo), the Gas Gun Relocation Project Team, the Phoenix Mini-Generator Explosive Pulsed Power Development Team, the Advanced Certification Hydro Team, the W84 SS21 Project Team, the Collaborative Authorization Safety Basis Total Lifecyle Environment Project Team, and the Barolo Subcritical Experimental Series Team.

In addition, WCI's Don Roberts became the latest recipient of the NNSA Defense Programs' Employee of the Quarter Award. Don was recognized for leading a multidisciplinary, international team in velocimetry pin testing in LLNL's Contained Firing Facility. The experiment studied what happens to metal adjacent to a high-explosive detonation. The multimillion-dollar test, conducted last October, culminated 3 years of work by a 44-person team of researchers from LLNL, the Nevada National Security Site, LANL, and the U.K.'s Atomic Weapons Establishment. Said Don Cook: "We are fortunate to have dedicated professionals who contribute directly to the many successes that NNSA Defense Programs have achieved this quarter. I am once again proud to praise the hard work being done by the men and women throughout the national security enterprise."

### About the Cover

Troy Barbee holds a multilayer coated grating developed at LLNL and used to capture the first-ever high-resolution, extreme-ultraviolet spectroscopic observations of binary white dwarf Feige 24. Troy won the Naval Research Laboratory's Alan Berman Research Publication Award in recognition for this work. (See "NRL award for white dwarf research," on page 2.)

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

## DTRA "TOP CONTRIBUTOR" AWARD FOR NUCLEAR FORENSICS

Geophysicist Arthur Rodgers received an award from the Defense Threat Reduction Agency (DTRA) for his work in nuclear forensics. Arthur was named "top contributor of the quarter" for the first quarter of fiscal 2012 for a forensic analysis project. As part of a DTRA program to develop methods for improved forensic analysis of signals from nuclear explosions, his LLNL team is developing the Integrated Yield Determination Tool, a software package that will be used to interpret prompt speed of sound data for explosion forensics. Said DTRA program leader Phil Cole, "Arthur and his team demonstrated the tool in October as part of an operational user assessment for STRATCOM and the test went very well," Phil said. "The test met the goals of the project and came in on schedule and on budget." Arthur said that while it is an honor to be recognized with the award by the DTRA program leadership, the award represents a credit to the entire team. "E.O. Lawrence founded this national laboratory on the basis of multidisciplinary teamwork. This project has succeeded because we can draw upon the expertise and diverse technical skills of different types of scientists and engineers," Arthur said.

## NRL AWARD FOR WHITE DWARF RESEARCH

Material scientist Troy Barbee is the most recent recipient of the Naval Research Laboratory's (NRL's) Alan Berman Research Publication Award for his work looking into the makeup of a white dwarf. The **paper**—the most recent publication stemming from a long history of collaboration between Troy and researchers in the NRL X-ray Astronomy Program and the University of Leicester—reports the first high-resolution spectroscopic observation of the binary white dwarf Feige 24 in the extreme-ultraviolent band. Troy used multilayer coated gratings developed at the Laboratory in the experiments. The findings show that helium is nearly completely lacking in Feige 24's makeup, a surprising result contrary to standard models of stellar atmosphere evolution. In the photo Troy holds one of the multilayer structures, which was fabricated in a high-vacuum magnetron sputter deposition apparatus. These wavelength-reflecting optics and nanolaminate materials are used for the scientific study of new phenomena and the development of advanced materials.

## New Inductee in County Women's Hall of Fame

Discovery of six new elements and other achievements earned Dawn Shaughnessy a place in the Alameda County Women's Hall of Fame for 2012. She was one of 11 women inducted at the 19th annual awards ceremony, held on March 31 in Oakland. In collaboration with scientists in Russia, the team led by Dawn discovered elements 113–118. She also led a group in proposing the name of the newest element to be officially accepted in the Periodic Table—element 116, which is set to be named Livermorium in honor of LLNL and the city of Livermore.

In addition to her research, Dawn thrives on getting young people interested in science. Her team recently received a $5,000 education grant for their research in discovering element 117 and donated it to Livermore High School's chemistry department. Dawn recalled how ill-equipped her high school chemistry class was and wanted to do something to help her community. Dawn and her achievements were recently **highlighted** by NBC affiliate KRON as part of its "Bay Area Proud" series.

## 94-Year-Old Researcher's "Drive to Discover" Profiled

ABC affiliate KGO TV **profiled** the Laboratory's Dick Post, "who at 94 is still cranking out patents and inventions" and "whose idea of retirement is coming into work only four days a week." The segment focuses on Dick's passive magnetic bearings and how he uses the technology to create "clever new energy sources," such as a flywheel made with carbon fiber. Also shown are mag-lev trains being developed at General Atomics with the technology. In the screen capture, Dick is discussing a device he works on with

Bob Yamamoto.

## U.S.-Japan Collaboration on Clean Energy

About 75 scientists from the United States and Japan gathered in February at the Pleasanton Hilton to participate in the U.S.-Japan Workshop on Clean Energy Technology. The three-day meeting grew out of a 2009 agreement between DOE and Japan's Ministry of Economy, Trade and Industry to collaborate on clean energy research. Said LLNL's Doug Rotman, the program director for Energy and Environmental Security in the Office of Strategic Outcomes, "We discussed the progress being made on clean energy projects using the unique facilities, staff, and capabilities in Japan and the U.S." Collaborative projects between the two nations are under way in solar energy, biomass, energy storage and nanomaterials, and other areas. "The thing that struck me about the conference," said Cesar Pruneda, a senior adviser in PLS, "was the outstanding research in both basic science and applied science being brought to bear by scientists from Japan and the U.S. on some very difficult energy challenges." The conference's plenary talk was delivered by Arun Majumdar, director of DOE's Advanced Research Projects Agency–Energy and nominee for Undersecretary of Energy. He spoke on the energy needs of the United States and DOE's strategy for delivering solutions. Dr. Majumdar spoke with Director Parney Albright and Deputy Director for Science and Technology Tomás Díaz de la Rubia and attended briefings on NIF, laser inertial fusion energy, and high-performance computing.

## Pathogen Detector Licensed

Livermore has licensed a microbial detection technology to St. Louis-based **MOgene LC**, a supplier of DNA microarrays and instruments. Known formerly as the Lawrence Livermore Microbial Detection Array (LLMDA), the technology could enable food safety professionals, law enforcement, medical professionals, and others to identify a pathogenic virus or bacteria within 24 hours. The LLMDA detects viruses and bacteria with the use of 388,000 probes that fit on a 1-by-3-inch glass slide. The current operational version of the LLMDA contains probes that can detect more than 2,200 viruses and 900 bacteria—essentially the entire range of known

viruses and bacteria—whereas previous multiplex polymerase chain reaction techniques can detect at most 50 organisms in a single test.

## NIF ACHIEVES RECORD LASER ENERGY

On March 15, NIF fired all 192 beams to deliver 1.875 million joules (MJ) of ultraviolet light to the target chamber's center, reaching 411 trillion watts of power and reaching a total energy of 2.03 MJ after passing through the final focusing lens. "This event marks a key milestone in the National Ignition Campaign's drive toward fusion ignition," said NIF Director Ed Moses. "While there have been many demonstrations of similar equivalent energy performance on individual beams or quads during the completion of the NIF project, this is the first time the full complement of 192 beams has operated at this energy. This is very exciting, like breaking the sound barrier." With these results, NIF is now the world's first 2-MJ ultraviolet laser, generating nearly

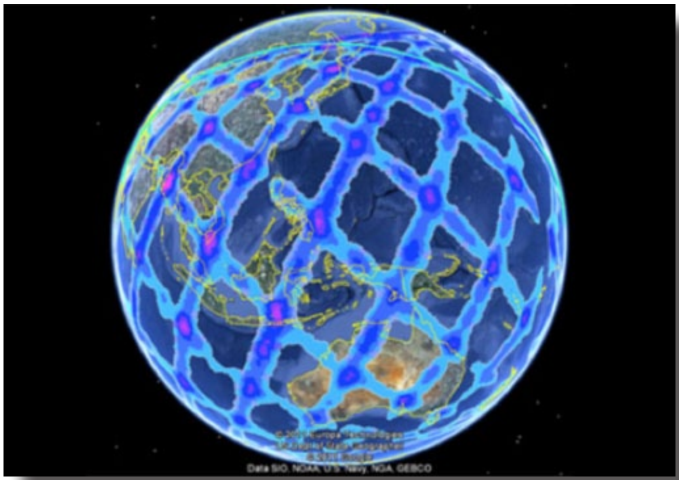

## TEST BAN TREATY REPORT, WRITTEN WITH LLNL INPUT, IS RELEASED

The National Research Council **report** *Comprehensive Nuclear Test Ban Treaty: Technical Issues for the United States* was publicly released on March 30. The report details the Committee's review and assessment of changes to technical issues that have occurred since the National Research Council's previous report on this topic in 2002. The report addresses the ability of the United States to maintain the safety and reliability of the U.S. nuclear stockpile; the capability to detect, locate, and identify nuclear explosions; commitments necessary to sustain the U.S. stockpile and the U.S. and international monitoring systems; and potential technical advances countries could achieve through evasive testing. LLNL Director Emeritus Bruce Tarter served on the main committee and PLS seismologist William Walter served on the seismic subcommittee. William and other committee members provided a classified pre-release briefing at the State Department on March 9 in Washington, D.C. William was also present for the public release on March 30.

## TEAM HELPS AIR FORCE TRACK SPACE DEBRIS

Lab computer scientists helped deploy the first production application of the Knowledge Assimilation and Reasoning for National Awareness of Counter-Space Threats Project into the Air Force's Integrated Web Space Situational Awareness System. The multilaboratory project provides the Air Force with critical information about the debris from the breakup of a satellite. Philip Edwards, Tim Bender, Josh Oakgrove, and JoAnne Levatin are contributing to the project. This team also leads the effort to integrate a complete enterprise application into the Joint Mission System to use on the floor of the Joint Space Operations Center (JSpOC).

The figure is a probability density map based on LLNL calculations—requested by JSpOC—indicating where the Russian Phobos-Grunt spacecraft could re-enter Earth's atmosphere. In this effort, Matt Horsley wrote initial Monte Carlo simulations of re-entry. Ben Fasenfest then developed a parallel version for UNIX, and the resulting model was used to provide real-time updates of the reentry prediction to JSpOC. The simulation predicted the reentry time within 20 minutes of the actual reentry on January 15. Livermore's NARAC had also been alerted to perform plume modeling in the event the fuel-laden craft had landed intact on land.




## NIF USER GROUP MEETING ATTENDED BY 20 NATIONS


Nearly 175 scientists, students, and postdoctoral researchers representing 20 nations attended the first NIF User Group meeting held at LLNL recently to discuss fundamental science research opportunities at NIF. After welcoming remarks by LLNL Director Parney Albright, an overview discussion of NIF science was held by NIF Director Ed Moses, senior DOE officials, and LANL's John Sarrao. Current and potential users in the self-organized user group then heard presentations covering the unprecedented power and precision of the NIF lasers, the facility's sophisticated diagnostic equipment, target fabrication and experimental platform capabilities, and the wide range of scientific experiments already under way or in preparation on NIF, as well as related research being performed at LLNL's Jupiter Laser Facility and the OMEGA laser at the University of Rochester. A poster session and a tour of NIF were also held. Chris Keane, director of the NIF User Office, led the local organizing effort for the meeting, along with Kim Hallock and Trina Voelker. Said Justin Wark, University of Oxford professor and NIF User Group interim chair, "The interest shown in using the NIF for basic science is evidence of the great enthusiasm that the academic base has for using such a unique machine, and their recognition that it will enable scientific inquiries that are simply impossible elsewhere."

## NEW FIBER DRAW TOWER COMMISSIONED

LLNL employees who participated in the design, procurement, assembly, and operation of the Laboratory's new optical fiber draw tower celebrated the facility's commissioning on February 21. The

8.2-meter-tall tower, which spans three floors in Bldg. 391, is capable of fabricating fibers ranging from 80 to 500 micrometers in diameter. Introducing the facility to NIF Director Ed Moses and other NIF managers, Gina Bonanno noted that LLNL now has a unique capability to design and model, as well as produce, various optical fiber structures on demand for a wide variety of research projects. Project leader Jay Dawson said the facility can reduce the time required to produce a new fiber design from four to five months to about a week. Gina credited the Laboratory's institutional funding with bringing the fiber draw tower capability to fruition. Pictured is John Tassano making an adjustment to the tower.

## COMPANIES CHOSEN FOR ACCESS TO LIVERMORE HPC

Six private-sector projects selected for the application of LLNL high-performance computing (HPC) were announced on March 20. Called the "**hpc4energy incubator**," this pilot program aims to accelerate the development of energy technology and boost U.S. competitiveness in the global marketplace by teaming industry with the scientific and computing resources at national laboratories. The companies selected span a broad range of industries—including drilling, electrical power generation, and automotive engineering—indicating the huge potential for using Livermore HPC to solve problems facing American business. These companies will collaborate with LLNL scientists and use Livermore's HPC to find solutions to urgent energy-related problems and learn how to employ HPC as a powerful tool for innovation. The projects will be managed by Livermore's **HPC Innovation Center**. "By bringing together industry's entrepreneurial know-how and the national labs' science and technology, we aim to establish a model for energy technology innovation," said Tomás Díaz de la Rubia, Deputy Director for Science and Technology. The hpc4energy incubator emerged from last year's National Summit on Advancing Clean Energy Technologies as a concrete means of boosting the competitiveness of American companies in the global energy market by using HPC to accelerate the development of new energy technologies.

## RESEARCHER SERVES ON RADIOANALYTICAL CHEMISTRY CONFERENCE COMMITTEE

Annie Kersting served on the organizing committee of the 9th International Conference on Methods and Applications of Radioanalytical Chemistry, **held** March 25–30 in Kona, Hawaii. Topics covered at this conference include nuclear forensics, the Fukishima disaster, environmental radiochemistry, and nonproliferation. Annie and Roger Martinelli both chaired sessions, and 13 Lab researchers gave either oral or poster presentations.

## RESEARCHERS GIVE INVITED KEYNOTES

Ilya Lomov was an invited keynote speaker at the International Symposium on Plasticity, held in San Juan, Puerto Rico, on January 3–8. Ilya presented research on the integration of mesoscale simulations with experimental work to support the continuum modeling of failure mechanics and inelastic behavior in granular materials.

In addition, Tarabay Antoun gave an invited presentation titled "Mesoscale Modeling of the Dynamic Response of Armor Ceramics" at the American Ceramic Society's 36th International Conference on Advanced Ceramics and Composites, held in Daytona Beach, FL, on January 22–27. Mesoscale modeling covers a large spectrum of deformation histories, from simple representative volume studies to direct simulations of complicated pressure-shear experiments. Simulations reveal a number of unconventional effects in particulate matter, such as post-shock shear stress relaxation and deformation-induced anisotropy, that are hard to detect experimentally. Analyses of microscale material response have already yielded enhancements to engineering material models.

## RESEARCHER JOINS NAVAL STUDIES BOARD

Tammy Jernigan was recently appointed by the National Academy of Sciences (NAS) to serve on the Naval Studies Board (NSB). The mission of the NSB, created in 1974, is to be a source of independent, long-range, scientific and technical planning advice for Naval forces. The NSB charter also was endorsed by the Assistant Secretary of the Navy (Research and Development), and accepted without modification by the president of the NAS and chair of the National Research Council.

## LIVERMORE FEATURED IN NOVA SHOW ON NEW ELEMENTS

The Laboratory was recently featured on NOVA's "Hunting the Elements," a 2-hour special in the *Making Stuff* series, hosted by David Pogue, technology correspondent of the *New York Times*. The Center for Accelerator Mass Spectrometry (CAMS) is featured as the scientists there use isotopes of carbon to date ancient items as well as identify some of the causes of global warming. A section on NIF focuses on the use of hydrogen in an attempt to create fusion energy. (A "sneak preview" of this section **was shown** on CBS Sunday Morning News.) Finally, Lab heavy element guru Ken Moody talks about the process of discovering the heaviest elements known to man. The screen capture shows physicist Tom Brown explaining how carbon dating works at CAMS.

## INVITED PRESENTATIONS AT APS MEETING

Nir Goldman and Mike Armstrong, both of PLS, gave invited presentations in the Materials at Extreme Conditions Symposium at the American Physical Society Meeting, held in Boston, MA, from February 28 to March 2. Nir presented a new approach to simulate matter under extreme conditions that is up to 100 times faster than the standard density functional molecular dynamics methods and demonstrated that his technique could accurately model NIF experiments performed on diamond. Mike presented a new technique combining dynamic compression in a diamond anvil cell with picosecond time-resolved diagnostics and discussed ultrahigh-elastic precursors in metals, as well as picosecond chemical dynamics in shocked liquids and explosives. Experiments using the dynamic compression technique on deuterium showed evidence of a ramp wave to shock transition that occurs in less than 100 ps.

## LLNL PERISCOPE INSTALLED ON DIII-D TOKAMAK

During the last week of January, a new LLNL-designed, wide-angle periscope system was installed on the DIII-D tokamak at General Atomics in San Diego. The periscope is based on a design that LLNL had previously developed for the ITER tokamak in France. The mirror box protects a main mirror assembly from the tokamak plasma, and enables a very wide view of the interior of the tokamak. The optical system images both infrared and visible light, so both the temperature of the vessel walls and plasma emission can be measured simultaneously. The DIII-D tokamak, which has been off line since last December for upgrades and the installation of new diagnostics, will resume experiments in May.

## LAB CO-SPONSORS NORTH DAKOTA ENERGY TECHNOLOGY SYMPOSIUM

Laboratory Deputy Directory for Science and Technology Tomás Díaz de la Rubia delivered the keynote address at the North Dakota Energy Symposium on Using Technology to Enhance Clean Energy Production, held March 5 at North Dakota State University. In his address at the event, which the Lab co-sponsored with the Howard Baker Forum and the university and which was hosted by Senator John Hoeven of North Dakota, Tomás stressed how high-performance computing (HPC) modeling and simulation can accelerate the development of clean energy technologies. EmPower ND, North Dakota's comprehensive energy policy, provided the framework for the symposium, which brought together energy experts from academia as well as government and industry. Discussion centered on opportunities and challenges in current methods of energy production, including how HPC represents an important tool for the private and public sectors to use in addressing those challenges.

## NONPROLIFERATION SPECIALIST GIVES LECTURE AT SONOMA STATE

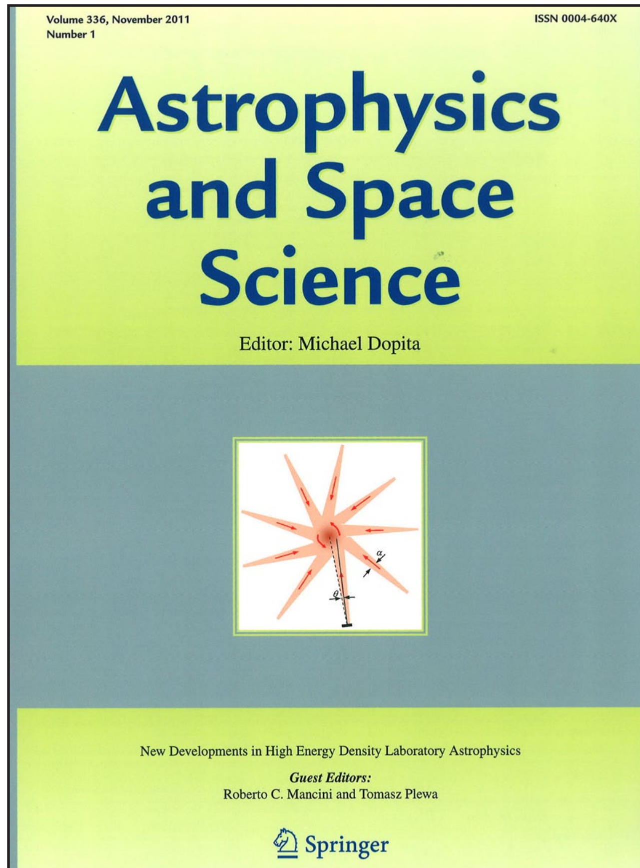
Carolyn Mac Kenzie (PLS) was a featured speaker in the "What Physicists Do" lecture series at Sonoma State University on February 13. In her talk, titled "Practicing Health Physics Around the World," Carolyn described her nonproliferation efforts for the International Atomic Energy Agency to locate and secure radioactive sources in developing countries, which often have no storage or disposal capabilities. She is now also involved in developing a training program for inspectors from the Comprehensive Test Ban Treaty Organization. After the lecture, Carolyn was **interviewed** by Bruce Robinson of KRCB radio.

## SDAV CHOSEN TO SUPPORT OFFICE OF SCIENCE

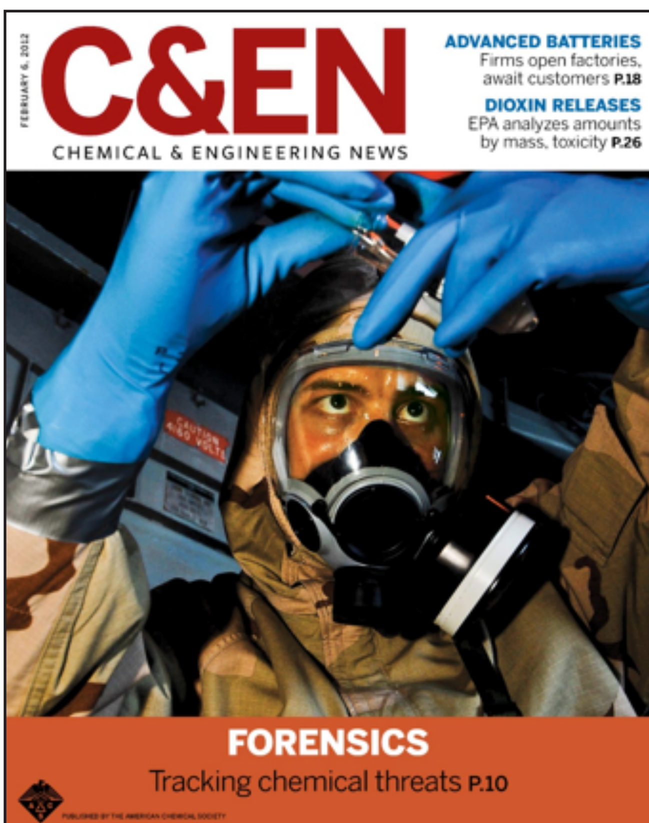
The DOE Office of Science's Advanced Scientific Computing Research Program chose the Scalable Data Management, Analysis, and Visualization (**SDAV**) Institute—of which LLNL is a member—to provide collaborators with more effective and efficient ways to manage, analyze, visualize, and understand their scientific data. Energy Secretary Steven Chu announced SDAV as part of the Obama Administration's Big Data Research and Development Initiative. The SDAV Institute, led by LBNL, is made up of more than a dozen national laboratories and universities and is funded at $5 million per year for 5 years. SDAV will help application teams achieve breakthrough science and provide solutions in the data management, analysis, and visualization regimes that are broadly used by the computational science community. The LLNL team will focus on deploying solutions to customers within the VisIt visualization and analysis tool. Eric Brugger is LLNL's principal investigator for the SDAV Institute.

## PAPER "COVERED" BY HED ISSUE OF *ASTROPHYSICS AND SPACE SCIENCE*

The November 2011 issue of *Astrophysics and Space Science* featured on its cover a paper by PLS researcher Dmitri Ryutov. The **paper**—"Using intense lasers to simulate aspects of accretion disks and outflows in astrophysics"—describes how some aspects of accretion disc physics can be experimentally simulated by using an array of properly directed plasma jets created by intense laser beams. Dmitri discusses how to create a quasi-planar disc with a Reynolds number exceeding 104 and a magnetic Reynolds number in the range of 10–100. This issue of the journal was a special issue devoted to current and future high-energy-density physics experiments relevant to astrophysics research and contained several papers by LLNL authors.



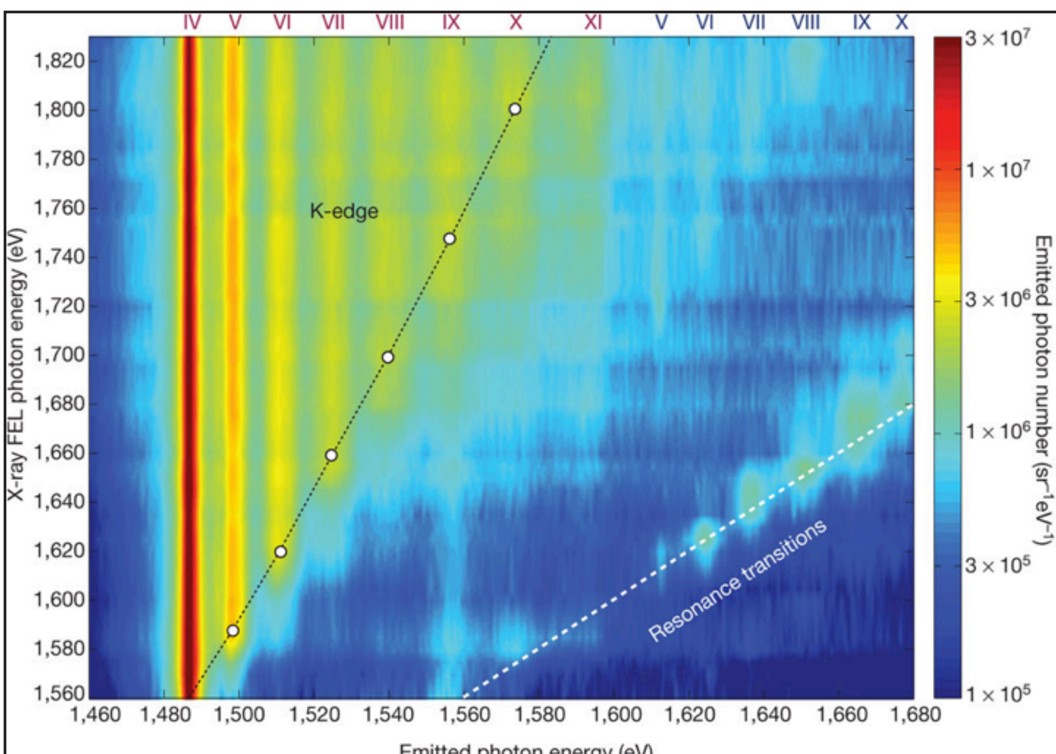

## WORK FEATURED AS *CHEMICAL & ENGINEERING NEWS* COVER STORY



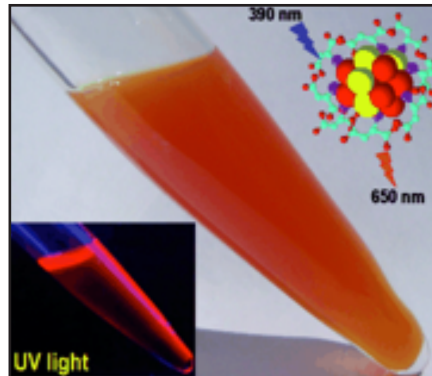

Work by Michael Singleton and Saphon Hok on using forensics to track chemical warfare agents was featured on the cover of the **February 6 issue** of *Chemical & Engineering News*. Saphon, in collaboration with the Swedish Defense Research Agency, has been using impurity profiling to link chemical threat agents to the methods used to make them. He analyzes the compounds using mass spectrometry and nuclear magnetic resonance spectroscopy to find signatures that pinpoint the production method used. Michael and Lab colleague Alan Volpe recently used stable isotope analyses to investigate the toxic industrial chemical ammonium metavanadate and the rodenticide tetramethylenedisulfotetramine, commonly known as TETS. In the case of the former, Michael and team purchased 19 samples from different suppliers and analyzed their nitrogen, hydrogen, and oxygen isotopic compositions. They determined that those 19 samples originated from six sources, which they were able to differentiate with "a very high level of confidence."

## *NATURE* PAPER ON PROBING SOLID-DENSITY PLASMA WITH X-RAY LASER

In a **paper** appearing in *Nature*, an international team of researchers, including PLS scientist Yuan Ping, report on the experimental creation of a solid-density plasma at temperatures in excess of 106 K on inertial-confinement timescales using the Linac Coherent Light Source x-ray laser. The paper discusses the physics of the intense x-ray–matter interactions, and highlights the importance of electron–ion collisions. Detailed simulations of the interaction process conducted with a radiative-collisional code showed good qualitative agreement with the experimental results. The results of this study will inform future high-intensity x-ray experiments involving dense samples, such as the coherent x-ray diffractive imaging of biological systems, material science investigations, and the study of matter in extreme conditions. The figure, plotting spectrally resolved K-alpha emission as a function of the x-ray free-electron laser excitation photon energy, shows that the main K-alpha peaks around 1,487 eV, followed by a series of peaks corresponding to emission from higher charge states due to a growing number of L-shell holes.

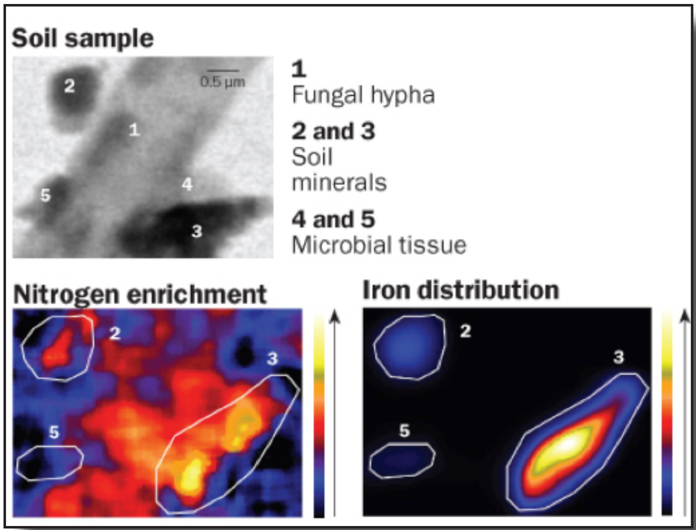



## "HOT PAPER" ON ALLOY QUANTUM CLUSTER




A **paper** by Krishnan Balasubramanian and colleagues from the Indian Institute of Technology, the S. N. Bose National Center for Basic Sciences, and the California State University East Bay was selected as a "hot paper" by *Angewandte Chemie* and published online on January 20. The team studied aluminum–gold mixed-metal clusters, a new category of alloy with unusual structures and properties and which may exhibit synergistic effects important in the development of novel catalysts. An alloy cluster containing a 13-atom core was synthesized from silver clusters via a galvanic exchange reaction. The alloy cluster shows luminescence with a quantum yield of 3.5% at room temperature, several times higher than the parent clusters. The figure shows the alloy's luminescence and the distorted icosahedral core suggested by their calculations.

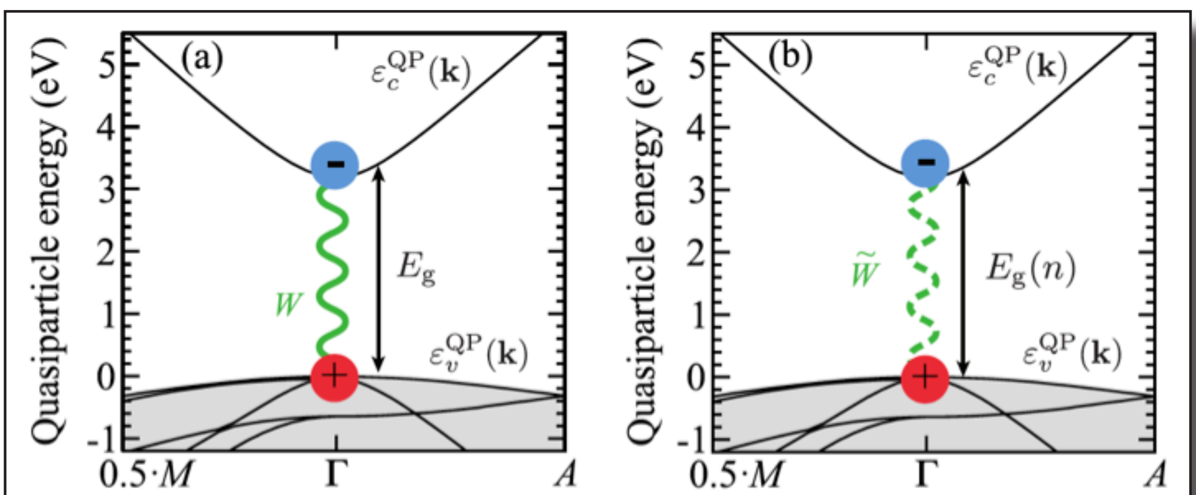
## SOIL RESEARCH IN *SCIENCE NEWS*




Work conducted at LLNL by Jennifer Pett-Ridge, Marco Keiluweit (a Lawrence Scholar and Oregon State University graduate student), Jeremy Bougoure, and Peter Weber using high-resolution imaging mass spectroscopy to investigate the biogeochemical cycling of carbon and nitrogen in soil was highlighted in an **article** entitled "Soil's hidden secrets," published in the January 28 edition of *Science News*. With support from Livermore's LDRD Program, and in collaboration with Oregon State University and LBNL, the Livermore team demonstrated a new way to visualize the incorporation of carbon-13- and nitrogen-15-labeled microbial cell residues onto the minerals in soil and thus better understand the dynamics of organic matter turnover. In the image featured in *Science News*, a fungal hypha sits amidst soil minerals and microbial tissues. The correlated nitrogen-15 and iron ion images suggest that nitrogen from fungal cell walls is digested by microbes and preferentially deposited on the surfaces of iron oxide minerals or coatings.

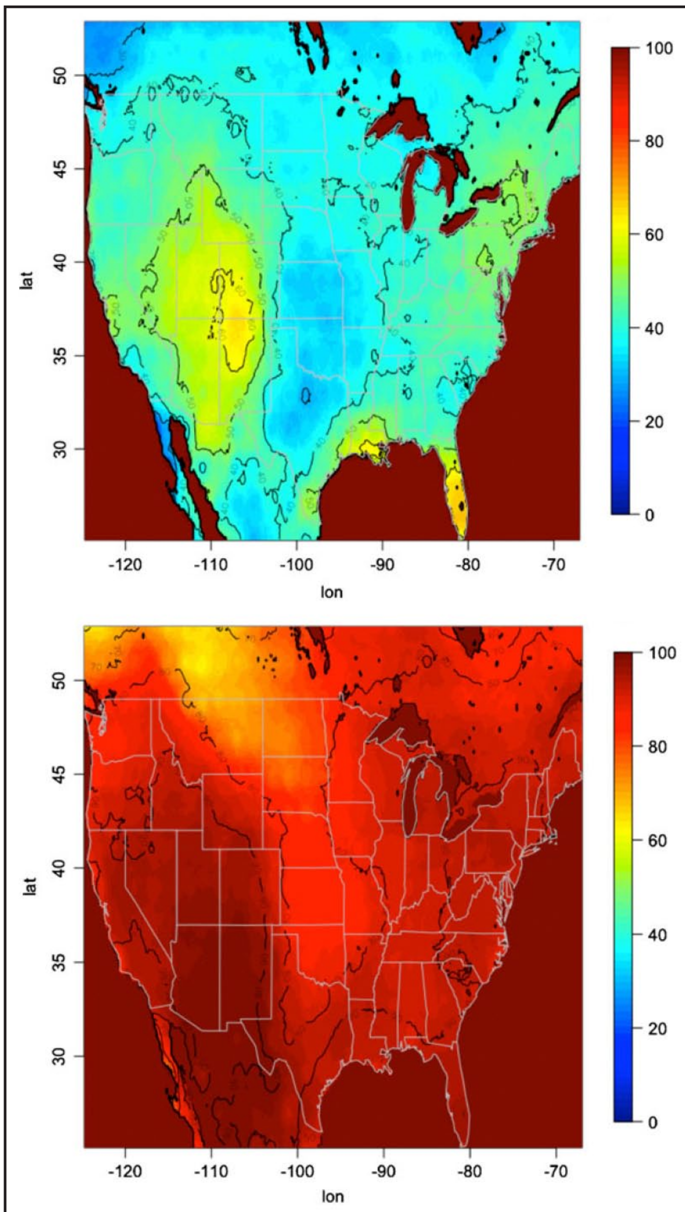
## POSTDOC PUBLISHES ON DEGENERATELY DOPED SEMICONDUCTORS

In a paper in *Physical Review Letters*, postdoc Andre Schleife **describes** a new approach he and colleagues developed to investigate the interplay of excitonic effects and electron doping. These interactions are critical to learning more about transparent conducting oxides (TCOs), which are used in a range of fields, including green energy, intelligent materials, and flexible and transparent electronics, such as car windows that also function as displays. "Successfully exploiting and eventually tailoring the properties of these unique materials would be analogous to creating 'transparent gold' with a plethora of technical applications," Schleife said. Excitons are the most important pair excitations that occur in several optical spectroscopies of nonmetals and molecules and dominate the absorption properties of the TCOs. The figure illustrates the free-carrier-induced effects on electron-hole pair excitations near the fundamental band gap of ZnO, comparing (a) electron–hole interaction (solid green wavy line) in the undoped material and (b) additional free-carrier screening affecting electron–hole attraction (dashed green wavy line).



## EXTREME TEMPERATURES WILL BE THE NORM: STUDY

By analyzing observations and results obtained from climate models, a study led by Phil Duffy and **published** in the journal *Climate Change* showed that previously rare high summertime temperatures are already occurring more frequently in some regions of the 48 contiguous United States. "The observed increase in the frequency of previously rare summertime-average temperatures is more consistent with the consequences of increasing greenhouse gas concentrations than with the effects of natural climate variability," said Phil, who is the lead author of the paper. "It is extremely unlikely that the observed increase has happened through chance alone." The geographical patterns of increases in extreme summer temperatures that appear in observations are consistent with those that are seen in climate model simulations of the 20th century. The figure shows the frequency with which summer-mean temperatures that were 95th percentile in the period 1950–1974 were exceeded by model-calculated data for the period 1995–2024 (top) and for the period 2035–2064 (bottom).

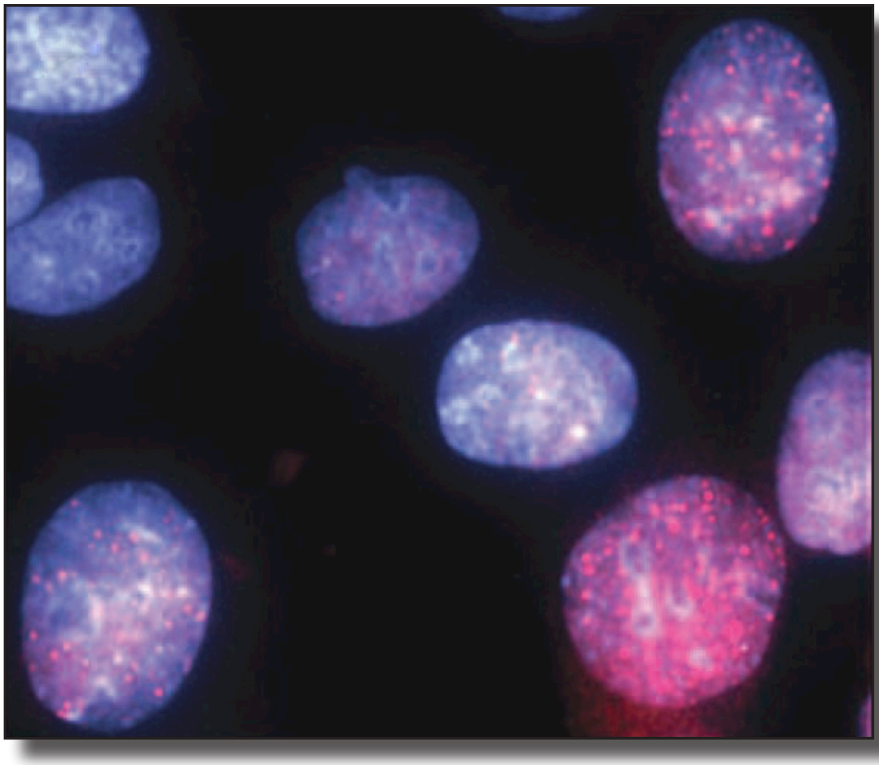



## PREDICTING STRUCTURE AND PROPERTIES OF CORRELATED-ELECTRON METALS

In a **paper** published in *Physical Review B*, the Laboratory's Per Söderlind, Blazej Grabowski, Lin Yang, and Alex Landa, along with colleagues from Aalto University (Finland) and Uppsala University (Sweden), show that use of the recently developed self-consistent ab initio lattice dynamics method, in conjunction with highly accurate and fully relativistic density functional theory (DFT), can overcome the limitations of conventional DFT, which are particularly problematic when an element's high-temperature phase is mechanically unstable at low temperatures, making it impossible to use perturbation methods for approximating the effect of higher temperature on structure. Using their new method, Per and colleagues show it is possible to predict the high-temperature (>1000 K) stable structure, phonon dispersion, and density of states for uranium, a prototypical actinide, obtaining results that compare well with experimental data. This result establishes that high-temperature lattice dynamics can be modeled from ab initio theory, even for complex materials with significant electron correlations such as the actinides. This work was supported by the Lab's LDRD Program and by the Computational Grand Challenge Program, which provided access to computational resources.

## UNRAVELING THE MECHANISMS OF DNA REPAIR

In a **paper** called out as an "Editors' Choice" and featured on the cover of the March 2012 **issue** of *Environmental and Molecular Mutagenesis*, Salustra Urbin, Larry Thompson, then-LLNL employee John Hinz, and colleagues from Stockholm University, report on the RAD51 family of related proteins that make up part of the cellular machinery that repairs dangerous double-strand breaks in DNA using the homologous recombination repair pathway. Following exposure of cells to these agents, RAD51 proteins localize within "nuclear foci," which are thought to be places of homologous recombination repair activity. The authors were able to demonstrate that cells lacking the RAD51D protein were defective in focus formation, but did not show cell killing by a chemical that arrests replication—demonstrating, for the first time, that cell survival and RAD51 focus formation can be separated as distinct cellular properties impacted by the RAD51 gene family of proteins. The figure indicates Distribution of RAD51 foci in stained irs1 *xrcc2* nuclei 20 hours after exposure to hydroxyurea.



## FIRST-PRINCIPLES SIMULATIONS OF NERVE AGENT REACTION PATHWAYS

Richard Gee, I-Feng (Will) Kuo, Sarah Chinn, and Ellen Raber were the authors of a **paper** describing first-principles molecular dynamics simulations of condensed-phase decontamination reactions of V-type nerve agent in an aqueous solvent. The paper, published in *Physical Chemistry Chemical Physics*, documents the results of a detailed study of hydrolysis, base-hydrolysis, and nucleophilic oxidation of both VX and R-VX, as well as their protonated counterparts. The decontamination mechanisms and chemical reaction energy barriers, as determined from simulations, were found to be in good agreement with experiment. The results demonstrate the applicability of using such simulations to understanding new decontamination techniques or, indeed, any other application that require computational screening of condensed-phase chemical reaction mechanisms. The paper was **highlighted** in an issue of the Royal Society of Chemistry's monthly magazine, *Chemistry World*.

## IMAGE-PROCESSING BOOK COAUTHORED

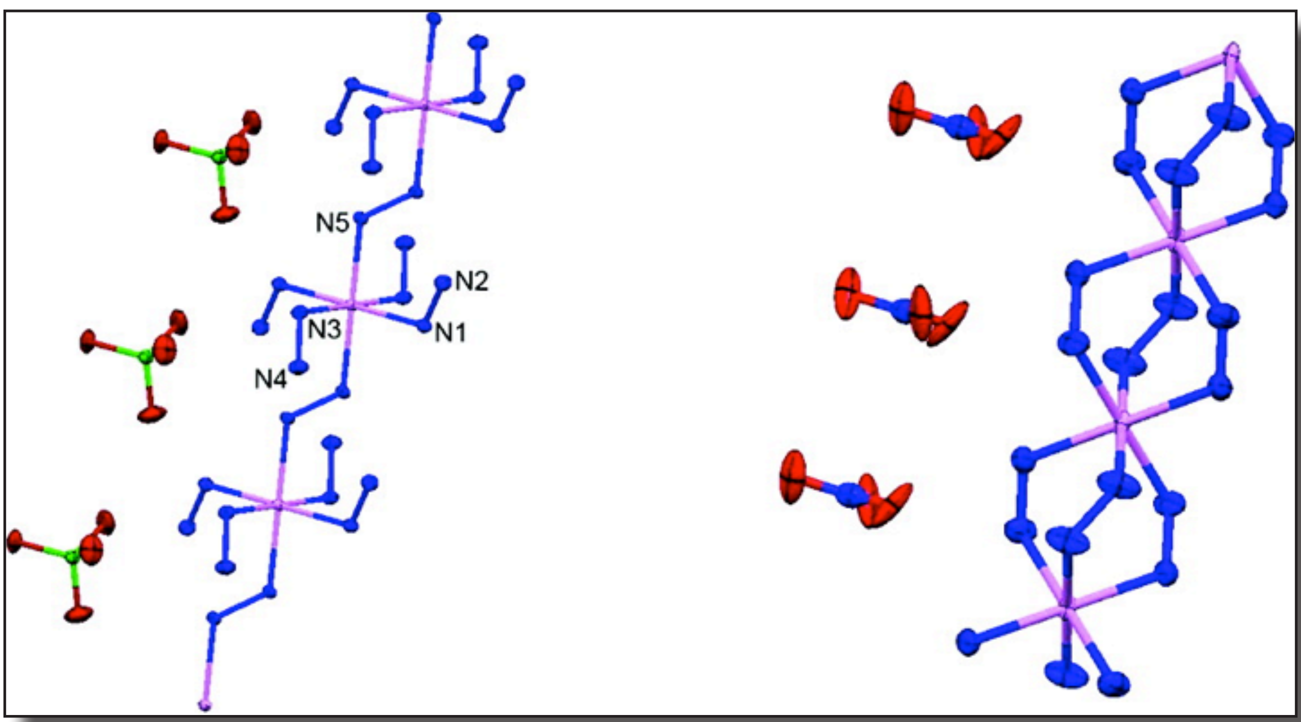
Abdul Awwal, of Engineering, coauthored a book entitled ***Field Guide to Image Processing***, which was recently published by SPIE Press. The book serves as a resource for commonly used image-processing concepts and tools. With this foundation, readers will better understand how to apply these tools to various problems encountered in the field. Topics include filtering, time-frequency-domain processing, image compression, morphology, and restoration. Abdul is a fellow of SPIE and OSA and will serve as conference chair for the next SPIE Photonics West conference, which will be held February 2–7, 2013.

## CHEMIST GUEST-EDITS SPECIAL ISSUE OF JOURNAL

M. Riad Manaa (PLS) and Yang Song, from the University of West Ontario, were guest editors of a **special issue** of the *Journal of Physical Chemistry C*. The issue contains articles summarizing research presented at the first symposium on the chemistry and materials science at high pressure, held at the Pacifichem Conference in Honulu, HI, December 18–19, 2010. A preface by the two describes new trends in chemistry and materials science in extremely tight space, including the discovery of exotic structures and properties, new classes of inorganic materials with unusual stoichiometries and crystal structures, and the high-pressure synthesis of new functional materials with industrial applications, such as superhard materials and hydrogen storage. The issue also features research articles by Riad and LLNL colleagues Larry Fried and Nir Goldman on nearly equivalent inter- and intra-molecular hydrogen bonding in 1,3,5-triamino-2,4,6-trinitrobenzene at high pressure and on the extension of density functional tight binding to carbon under extreme conditions.

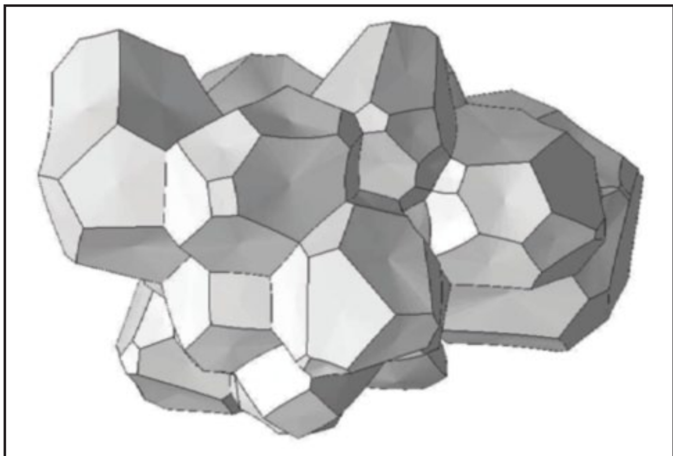
## NEW METAL-BASED EXPLOSIVE POSSIBLY MOST POWER EVER

Amitesh Maiti and Richard Gee, in collaboration with colleagues from Texas Tech University, used a combination of synthetic chemistry and computations to find new nickel- and cobalt-based energetic materials with high energy content and novel polymeric structures. Their results were **published** in the *Journal of the American Chemical Society*. Energetic materials have been used for nearly two centuries by the military and industry. Nevertheless, there has been little advancement in the development of completely new energetic motifs, despite longstanding research efforts to develop superior materials. The article reports on the discovery of new energetic compounds of exceptionally high energy content and novel polymeric structure that avoid the use of the lead and mercury salts common in conventional explosives. Laboratory tests indicate the remarkable performance of these nickel- and cobalt-based energetic materials, and density functional theory calculations indicate these are possibly the most powerful metal-based energetic materials known to date. The figure shows the structure of two compounds studies, with ellipsoids scaled at 50% probability.



## POSTDOC'S PAPERS HIGHLIGHTED

Jeremy Mason, a postdoc in PLS, has had two of his recent papers highlighted by the journals in which they appeared. The **first paper** provides an explanation for the Law of Aboav-Weaire, a simple mathematical expression derived from the empirical observation that in both two- and three-dimensional aggregates of grains, those grains with a small number of sides tended to be surrounded by grains with a

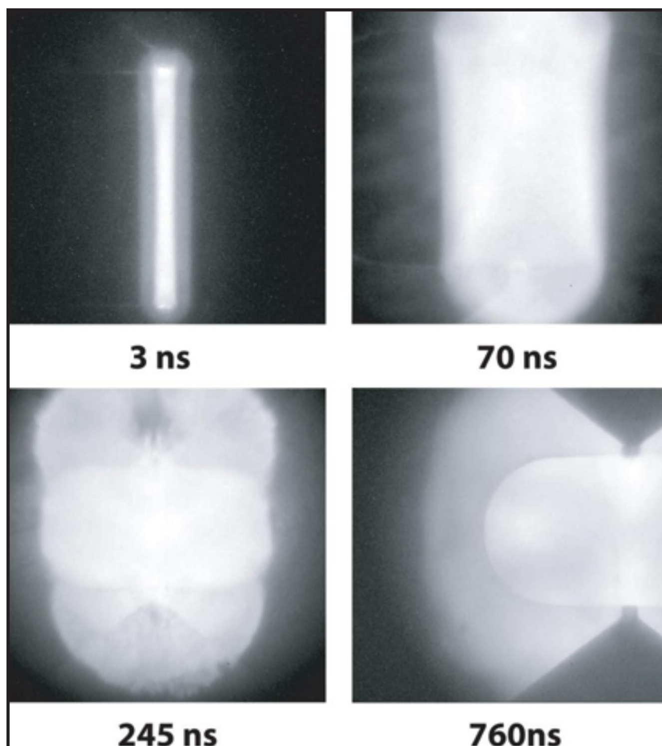


large number of sides, and vice-versa. Jeremy's paper provides an exact derivation of the mathematical form of the law and establishes a connection between the number of faces of a grain and the total Gaussian curvature contained in the faces and the edges of that grain. This paper was **featured** in the "Insights" section of the *Journal of Physics A*. The figure, from this paper, shows a collection of bubbles indicating the structural features of a cell complex, of which a grain is the basic three-dimensional constituent.

The **second featured paper** discusses the complexities of the topology of packing of disks in two dimensions and was selected for the January 2012 "Kaleidoscope" section of the *Physical Review E* website. The configuration space of hard disks is not known explicitly but is important to many questions in statistical mechanics, including the solid–liquid melting transition. Jeremy and his coauthors from Stanford University and the Institute for Advanced Study in Princeton studied the configuration space for five disks in the unit square using novel computational techniques and showed that mechanically balanced configurations act as "critical points"—the only places where the topology can change.

## RESOLVING PETN PATHWAYS

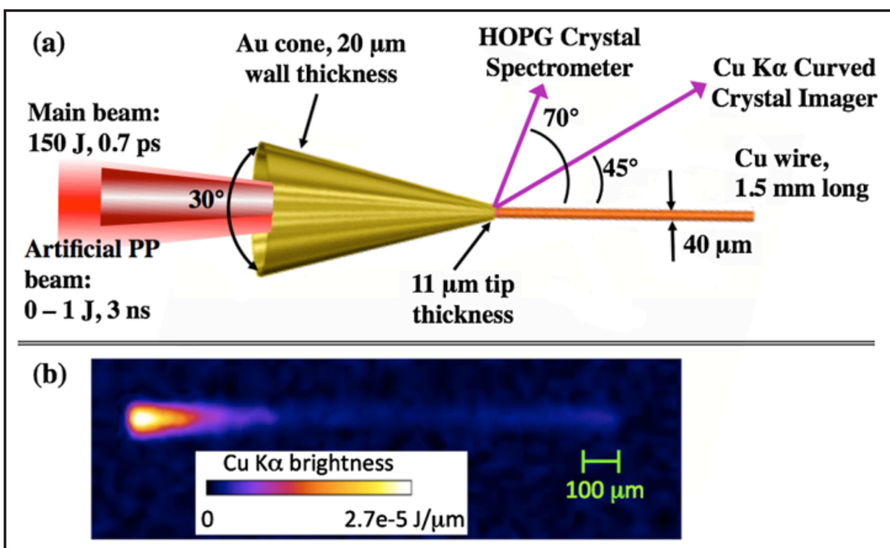
In a **recent paper** in the *Journal of Applied Physics*, Vincent Tang, Christian Grant, Jim McCarrick, Joseph Zaug, Elizabeth Glascoe, and Han Wang report on the spark initiation of the explosive pentaerythritol tetranitrate and the plastic poly(methyl methacrylate). The study temporally and spatially resolved plasma temperatures and electron densities (with atomic emission spectroscopy) and hydrodynamics (from fast, visible imaging) to gain a scientific understanding of an important safety issue. No methodology currently exists for the first-principles evaluation of arc initiation of high explosives, in spite of a critical need to evaluate low-probability but high-consequence accidents involving munitions. The figures

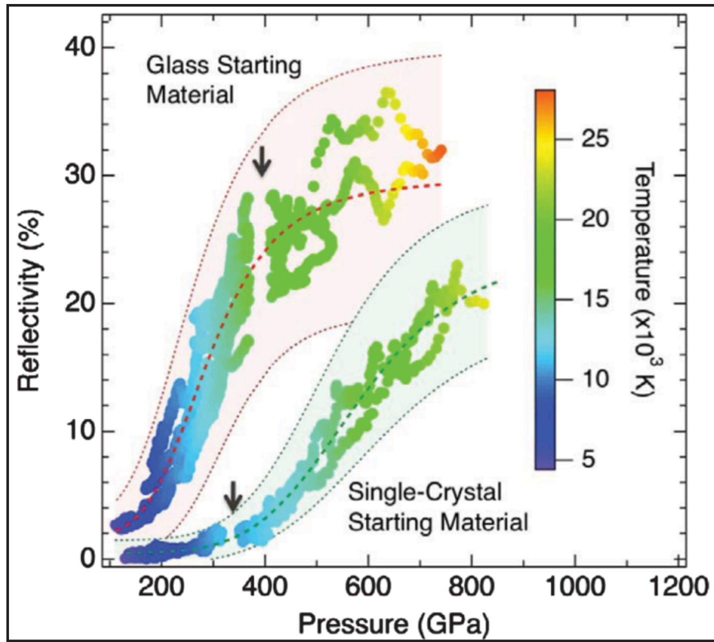



are fast-gated images at four different times with a 2-ns gate width. The bright, hot plasma kernel is easily discerned from the cooler, denser shock front that emits less visibly.

## PAPER EXPLORES "HOT" ELECTRONS FOR FAST IGNITION

In a **paper** chosen as an "Editor's Suggestion" in *Physical Review Letters*, Livermore's Tammy Ma and colleagues at LLNL, UC San Diego, Ohio State University, and General Atomics describes a possible approach for tailoring a laser-generated stream of energetic ("hot") electrons for achieving fast ignition in inertial confinement fusion capsules. The approach would generate the hot electrons at the tip of a hollow cone embedded in the capsule and so is known as cone-guided fast ignition. To examine the effect of increasing prepulse energy on the energy spectrum and directionality of the hot electrons, the team used simulations and experiments performed on the Titan laser, finding that the overall conversion efficiency of laser light into electrons that could potentially contribute to the ignition of a precompressed fuel capsule fell as the prepulse energy rose. These and other results highlight the need to minimize prepulse levels to optimize the yield of hot electrons able to couple to the fuel. The figure shows (a) a schematic of the cone-and-wire target and diagnostic geometry and (b) an example of a spatially resolved image of K-alpha emission along the wire.



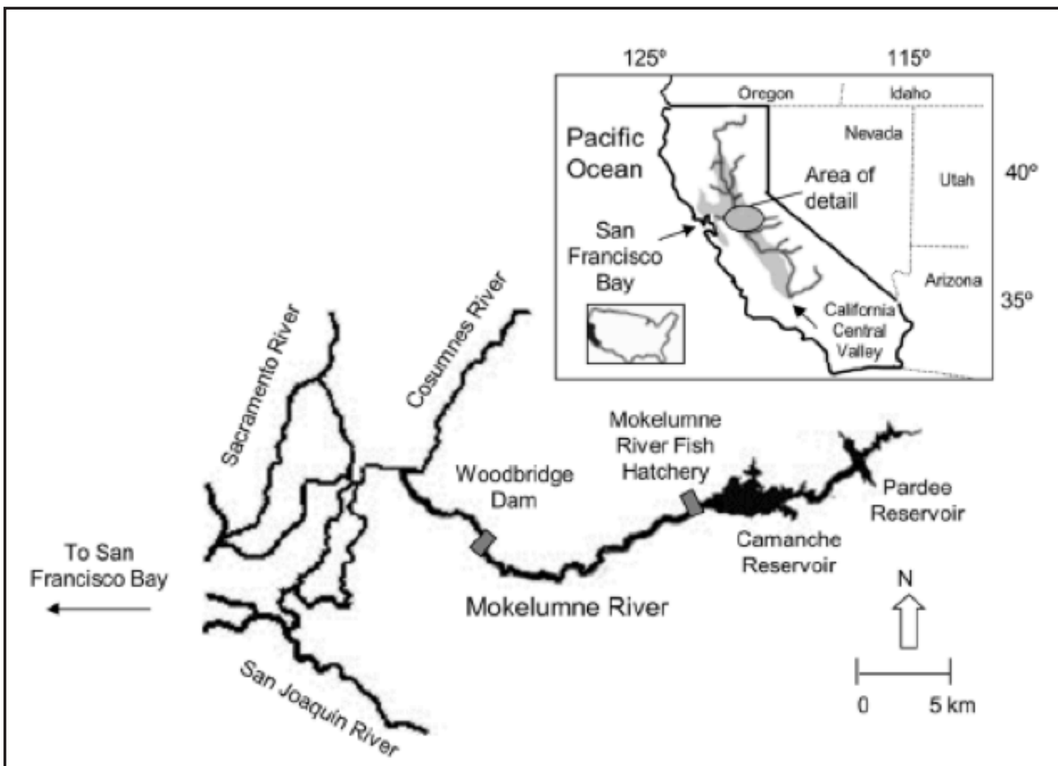




## LASER RESEARCH ELUCIDATES PLANET-FORMING PROCESSES

In work supported by LDRD and **reported** in *Physical Review Letters*, a team led by Dylan Spaulding—a UC Berkeley graduate student who conducted most of his thesis work at the Jupiter laser—used LLNL's Janus laser and OMEGA at the University of Rochester to conduct the experiments achieving the same extreme temperatures and pressures found in the interiors of exoplanets. A powerful laser pulse generated a shock wave through a sample, and by looking for changes in shock velocity and sample temperature, the team identified discontinuities signaling a phase change. They discovered that molten magnesium silicate abruptly transformed to a more dense liquid and concluded that such a liquid–liquid phase transition in silicate compositions could help explain the thermal-chemical evolution of exoplanet interiors. The figure graphs data showing the onset of metallization: reflectivities exceeding 5–10% indicate a gradual change in bonding character that is predominantly temperature driven.

## HATCHERIES LEAD TO GENETIC "SINKS": RESEARCH

A **new report** sheds light on the effects of hatchery fish on wild gene pools: only about 10 percent of the fall-run Chinook that spawn in the Mokelumne River are naturally born fish, indicating that all fish in the river have a parent or recent ancestor that came from a hatchery. The research team, made up of Laboratory scientist Peter Weber and collaborators, identified hatchery fish using a novel technique, developed in part at LLNL, that detects traces of a hatchery diet in the ear bones of adult fish. By analyzing the sulfur isotopes in the ear bones, called otoliths, which were deposited during their juvenile years, Peter and colleagues were able to determine whether individuals were produced in hatcheries or naturally in rivers. The result showed that only 10 percent of adults spawning in the river had otolith sulfur ratios characteristic of naturally produced salmon. It was the first time biologists were able to quantify the percentage of hatchery fish in this river, most of which are unmarked and therefore undetectable in population surveys. The research shows that wild Chinook salmon are not self-sustaining but rather represent a sink population when hatchery fish are taken into account. "It looked like a healthy population of fish returning to spawn, but the reality is that without the hatchery fish, the wild stocks are not sustaining themselves," said Rachel Johnson, the lead author and a fishery biologist affiliated with the Institute of Marine Sciences at UC Santa Cruz and with the U.S. Bureau of Reclamation.




## DISLOCATION DYNAMICS PAPER IS 8TH MOST DOWNLOADED FROM *ACTA MATERIALIA* IN 2011

A paper co-authored by PLS materials scientist Tom Arsenlis and Computation's Gregg Hommes and published last September in *Acta Materialia* was the 8th most downloaded **paper** from that journal for all of 2011. The paper reported on the use of the LLNL dislocation dynamics code, ParaDiS, to model the interactions of a dislocation with a low-angle grain boundary in a body-centered-cubic metal. Five different types of interactions were considered, and the overall resistance to transmission of the dislocation was calculated. These processes are important for understanding how the strength of metals change as a result of deformation.

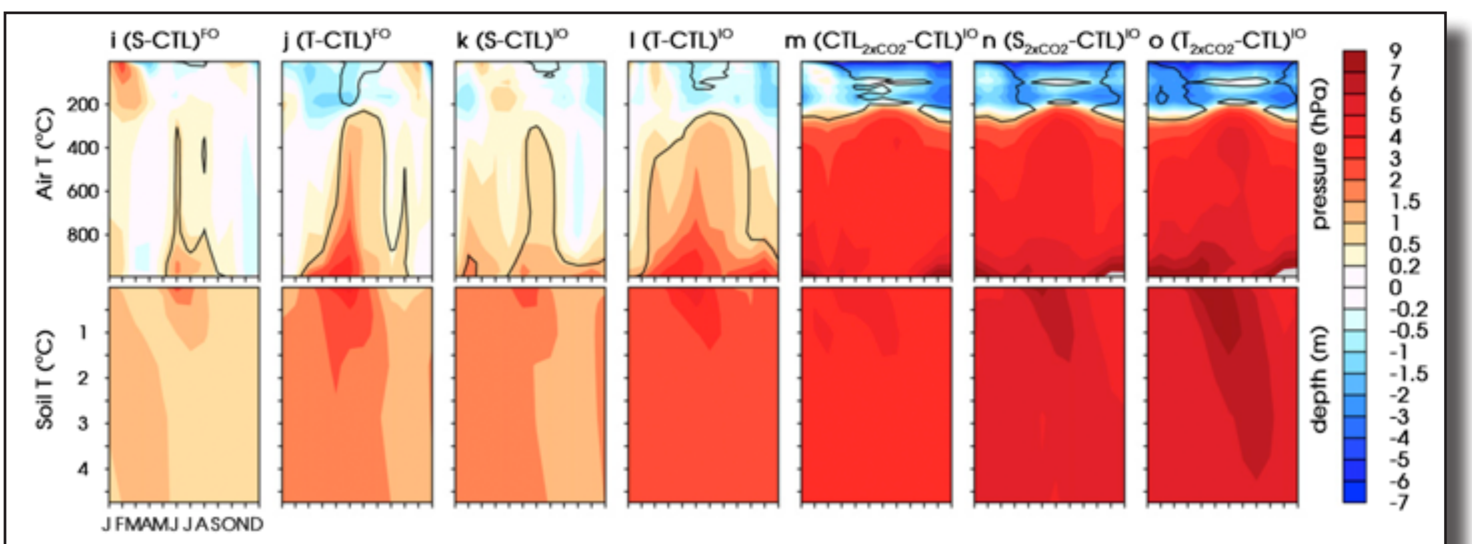
## CLIMATE EFFECTS OF EXPANDING BOREAL VEGETATION

Observational evidence indicates that trees and shrubs are invading tundra regions due to global warming at high latitudes. In a **paper** published in *Environmental Research Letters*, Livermore researchers Celine Bonfils, Tom Phillips, and Philip Cameron-Smith, with colleagues from LBNL and the National Center for Atmospheric Research (NCAR), present the results of computer simulations that indicate that an invasion of shrubs can further warm the northern high latitudes at a rate that depends on the height of the plants. The paper was also featured as a **news item** on the journal's website and in a "Perspectives" **commentary** in the journal.

In the paper, published as part of the journal's **Focus on Dynamics of Arctic and Sub-Arctic Vegetation**, the team describes a series of idealized computational "experiments" with the NCAR–DOE Community Climate System Model to investigate the impact of a potential large-scale tundra-to-shrub conversion on permafrost and the boreal climate. They found that increasing the total shrub fraction from 32% to 51% in the land north of 60°N triggered a substantial regional atmospheric warming in spring and summer because of reduction in the land–surface albedo and an increase in the water vapor content of the atmosphere because of increased transpiration. The team also found that the strength and timing of these two mechanisms depends strongly on the height of the shrubs, which controls the time at which branches and leaves protrude above the snow: taller and aerodynamically rougher shrubs lower the albedo earlier in the spring and transpire more efficiently than do shorter shrubs. This increases soil warming and destabilization of the permafrost. The figure shows an annual cycle of air and soil temperature as a function of height and depth for multiple simulations [(i) through (o)] relative to the control (CTL). The black line outlines statistically significant anomalies at the 99% confidence level.

## "OUTSTANDING REFEREES" RECOGNIZED BY APS

Livermore's Oleg Schilling and K.-T. Cheng were named by American Physical Society (APS) Editor-in-Chief Gene D. Sprouse as "outstanding referees" of *Physical Review* and *Physical Review Letters*. Under a program instituted in 2008 to recognize scientists who have been exceptionally helpful in assessing manuscripts for publication in the APS journals. By means of the program, APS expresses its appreciation to all referees, whose efforts in peer review not only keep the standards of the journals at a high level but in many cases also help authors to



improve the quality and readability of their articles—even those that are not published by APS. The highly selective Outstanding Referee Program annually recognizes only about 150 of the roughly 60,000 currently active referees. Like APS fellowships, this is a lifetime award. This year, 149 outstanding referees have been selected.

## WORK ON METHANE HYDRATES HIGHLIGHTED IN NETL NEWSLETTER

A **paper** by postdoc Wyatt Dufrane and colleagues from the U.S. Geological Survey and the Scripps Institution of Oceanography that appeared in the electronic edition of *Geophysical Research Letters* was also featured in *Fire in the Ice*, newsletter of the National Energy Technology Laboratory's Methane Hydrate R&D Program. The paper presents the first-ever electrical conductivity measurements on unmixed $CH_4$ hydrate and reported conductivity roughly five orders of magnitude lower than seawater. This difference allows electromagnetic (EM) techniques to distinguish highly resistive gas hydrate deposits from conductive water-saturated sediments in EM field surveys. This work was funded by DOE Methane Hydrates R&D Program in the Office of Fossil Energy. The figure compares inverted controlled source electromagnetic (CSEM) resistivity data to well log and seismic data at Hydrate Ridge, showing the potential of CSEM as a complementary geophysical method for gas hydrate assessment. The figure presents cryo-scanning electron microscope images, at different magnifications, of a mixture of sediment and single-phase (unmixed) polycrystalline $CH_4$ hydrate with 20% porosity.

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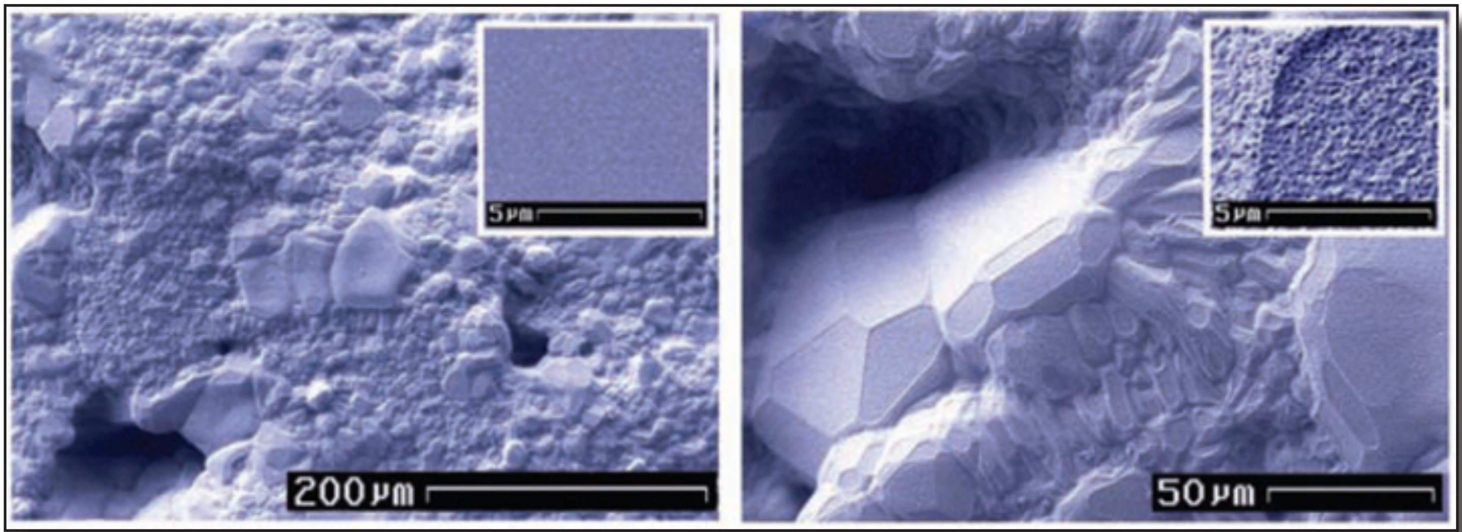

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**Questions? Comments?**
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