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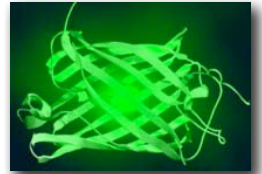
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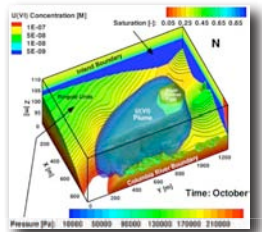
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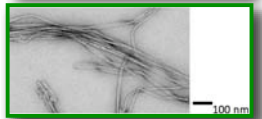
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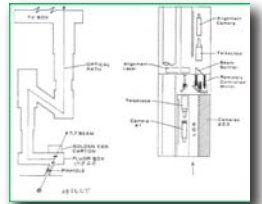
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PADSTE HIGHLIGHTS February 3, 2010

AWARDS

**Ricardo Lebensohn receives the Humboldt Research Award for senior US scientists**



Ricardo Lebensohn (MST-8) received a Humboldt Research Award for senior scientists. His citation reads, “He has pioneered the field of multiscale modeling of plasticity of crystalline materials, developing sophisticated theories and efficient numerical methods to connect the behavior of single crystals and polycrystalline aggregates, which are nowadays used by researchers worldwide, both for academic research and industrial applications.”

Lebensohn studies the structure/property relationships of materials. He coauthored the widely used ViscoPlastic Self-Consistent (VPSC) code to model the mechanical behavior and texture development of polycrystalline aggregates. Lebensohn recently developed a spectral method, which predicts the full micromechanical fields in deformed polycrystals. This method uses direct input from images of the material’s microstructure. His simulation tool complements novel three-dimensional, time-resolved techniques in experimental mechanics. Modeling structure/property relationships of polycrystalline materials enables revolutionary changes in the way simulations of the mechanical behavior of materials are performed, particularly for engineering applications. The interplay between microstructure and properties can be explicitly considered through fully-directional physically-based laws. Lebensohn has authored more than 90 international publications. He was a professor at the National University of Rosario (Argentina) and a researcher at Argentina's National Research Council before joining LANL in 2003.

The Alexander von Humboldt Foundation grants up to 100 Humboldt Research Awards annually. The award recognizes a researcher’s entire achievements of fundamental discoveries, new theories, or insights, which have had a significant impact on a scientific discipline. The Humboldt Foundation promotes academic cooperation between German scientists and colleagues from abroad. As part of the award, Lebensohn will spend several months in Germany collaborating with researchers at the Max-Planck Institute for Steel Research in Düsseldorf and the Fraunhofer Institute of Mechanics of Materials in Freiburg on projects of common interest.

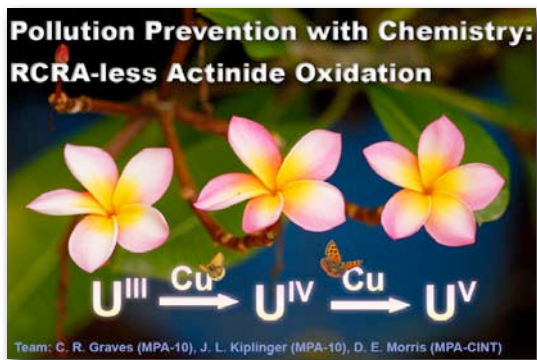
**LANL wins four NNSA Pollution Prevention Awards**

The awards are based on a NNSA-wide competition and recognize major contributions in pollution prevention, recycling, and procurement. The awards affirm the importance and benefits of integrating pollution prevention into all NNSA sites’ operations through environmental management systems.

***RCRA-less Oxidation* (NNSA Best in Class Award):** LANL developed a RCRA-less oxidation approach to replace toxic Resource Conservation and Recovery Act (RCRA)-listed salts with non-toxic reagents for actinide separation schemes. Historically, most actinide oxidation chemistry was performed using RCRA-listed silver and thallium salts. *RCRA-less Oxidation* demonstrates that simple copper (I) salts can provide simple chemical control over uranium (U) in a range of oxidation states. The large range of accessible oxidation states using a single nontoxic reagent is unprecedented and has potential for actinide separations schemes and advanced nuclear fuel cycles. The new copper-based oxidation

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protocol avoids the generation of mixed low-level radioactive hazardous waste and reduces labor hours and money spent in management of this waste stream.



*RCRA-less Oxidation* enables a 140-fold decrease in cost for waste treatment and disposal relative to other, standard oxidation methods. The process generates Low Level Rad Waste rather than mixed low-level radioactive hazardous waste. There is a 3-fold decrease in cost of raw starting materials because silver salts are more expensive than their copper analogues. Chris Graves and Jackie Kiplinger (MPA-CMMS), and David Morris (MPA-CINT) developed the process.

### ***Radiological Laboratory/Utility/Office Building (RLUOB) Integrated Planning, Design, Procurement, and Construction (NNSA Best in Class Award):***



LANL uses the LEED® third party rating system to document high performance sustainable design considerations and measure the level of sustainability that the RLUOB building achieves. Green design and implementation elements include sustainable site selection and development adjacent to programmatic facilities it will serve, construction with highly reflective roofing material to minimize the heat island effect, water efficiency, optimized energy performance, an indoor air quality management plan,

and reduced environmental impact of materials and resources. Through September 2009, approximately 85% (by weight) of RLUOB construction waste including concrete, metal, corrugated cardboard, wood, and asphalt were recycled or reused and thereby diverted from disposal in landfills. Lessons learned during RLUOB design and construction activities are being applied to other LANL projects. Award recipients are Rick Holmes, Nicole Seguin, and Don Shoemaker (CMRR-DO); Cathy Flavin (ES-PE); Joyce Matthew and Bob Ping (ASM-DEP); Steve Overton (CM-DO); Tony Ladino (PMF-MFG); Dave Tokach and Chandler Elkins (CM-STRS).

### ***LANL's Electronic Recycling Program (NNSA Environmental Stewardship Award):***



In the past, LANL disposed of computers by removing the hard-drives, shredding and disposing of them through an out-of-state electronic recycler. The computer shell was then released for sale to the public. LANL could not guarantee that the materials sold to the public would be managed appropriately, especially in light of rising concerns about electronics recycling in third world countries and associated pollution and public health issues. In addition, new memory device security requirements greatly expanded the types of electronic memory devices to include digital cameras, two-way radios, cell phones, and pagers, copiers, faxes, printers, PDAs,

iPods, phones, thumb drives, as well as circuit boards, computers, and laptops. Property management staff identified improvements to the process that improved security and closed the loop on all of LANL's salvaged memory devices, ensured proper cradle-to-grave management of LANL property through a zero-waste system, and reduced the operation's overall carbon footprint. In 2009, LANL shipped 93,554 lbs of e-waste to Terrell, TX. The estimated savings is for one year is \$172K. All of LANL's e-waste is recycled appropriately through this process. Award recipients are Charlotte Lindsey (OCIO), Melissa

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Metcalf (PS-1), John Tapia, Michael Shepherd, Mark Salazar, Mike Trujillo, and Rick Valerio (ASM-PM); Yvonne Gonzales (ASM-SBP); Barbara Martinez (ASM-PUR); and Earl Valdez (MSS-FEW).

**Alternative Fuel Use at LANL (NNSA Environmental Stewardship Award):** In FY 2009 a third of the LANL fleet could use E-85 fuel, which is an alcohol fuel mixture that typically contains up to 85% denatured fuel ethanol. In FY 2010, one-half of LANL's fleet of vehicles are flex-fuel. Currently, 75 percent of the SOC fleet in Los Alamos is powered by E-85. DOE Order 430.2B requires alternative fuel to be available within a five-mile radius of any DOE site. Since no local vendors have E-85 fuel available, Fleet Management procured a mobile E-85 fuel transport truck. The drivers of SOC flex-fuel vehicles requiring fuel are contacted by radio and asked to converge at a specified location for fueling. By using alternative fuels, LANL is meeting the intent of Executive Order 13423, Strengthening Federal Environmental, Energy, and Transportation Management, which led to DOE Order 430.2B. Award recipients are Dennis Bierer (SOC-LA), Andrew Erickson (UI-DO), Arlene Estevan, Jennifer Lucero, LeRoy Padilla, and John Tapia (ASM-PM); Paul Moore (COMPA); James Knotts (SOC-LA); and Tim Walker (MSS-HERG).



The Lab will issue the call for new Pollution Prevention nominations soon. LANL submits the best of these nominations to NNSA for their award consideration.

## ACCELERATOR OPERATIONS AND TECHNOLOGY

### LANSCE beam reliability achieves “world class” ranking

AOT has issued the CY2009 Los Alamos Neutron Science Center (LANSCE) Beam Report for cumulative reliability. The cumulative performance for CY2009 covers the period from June 2, 2009 through December 12, 2009. The results are displayed in the Table. The DOE Office of Science/Basic Energy Sciences considers a reliability standard of 85% to be “world class”.

**CY2009 LANSCE Beam Reliability Report**

<i>Experimental Facilities</i>	<i>Cumulative Reliability</i>
Manuel Lujan Center	85.25%
WNR Target 4	89.94%
Proton Radiography	91.74%
Isotope Production Facility	95.16%
Ultra-Cold Neutrons	84.79%
WNR Target 2	91.50%

LANSCE is a national resource that supports basic and applied research for national security and civilian applications. The heart of LANSCE is a highly flexible linear accelerator (linac) system, one of the most powerful in the world, that can accelerate up to 1 milliampere of protons to an energy of 800 million electron volts (MeV), and then deliver the protons to multiple experimental areas (Photo). The linac can also accelerate negative hydrogen ions to 800 MeV. The Isotope Production Facility uses protons at 100 MeV to make medical and other short-lived radioisotopes. The Proton Radiography Facility employs

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pulses of 800-MeV negative hydrogen ions to image dynamic events related to nuclear weapons performance. These pulses are also sent to heavy-metal targets at the Weapons Neutron Research (WNR) Facility, where proton–nucleus collisions in the targets generate large numbers of neutrons through a process called nuclear spallation. The neutron pulses are used for materials irradiation and nuclear science research. The negative hydrogen ions are also injected into the Proton Storage Ring, which compresses the 625-microsecond pulses into a 125-nanosecond (half-width at half-maximum) intense burst. Those intense proton bursts produce, through nuclear spallation, bursts of neutrons for neutron scattering studies of material properties at the Lujan Center and for nuclear physics research at the WNR. A newly commissioned ultracold neutron (UCN) research facility is exploring fundamental nuclear physics to test the standard model of elementary particles. LANSCE facilities are available to qualified scientists and engineers through a competitive proposal process. Each year LANSCE receives many more worthy proposals than it can accommodate. The scientists who conduct experiments at LANSCE represent a cross section of the research community—universities, industry, and national and federal laboratories—and come from all over the world.



Photo: Aerial view of LANSCE.

## BIOSCIENCE

### **Comprehensive analysis of filamentous phage display vectors for cytoplasmic proteins**

Most biological functions are initiated by or include the binding of molecules to targets to form molecular complexes. As such, developing new ways to mimic or exploit such binding is a critical component of bioscience research. Phage (short for *bacteriophage*) are simple viruses that infect bacteria and then hijack them so that they devote all their capacities to producing more phage. Scientists often use phage as tools in molecular biology. By adding additional genetic information to a phage (such as the gene for a specific protein X), it is possible to produce novel phage that will “display” the specific protein X on its surface. The protein X is then available to interact with its natural targets, and can be used to bind to and select for specific targets. However, this technology does not work very well with proteins that normally fold in the cytoplasm.

B-9 researchers (Nileena Velappan, Hugh Fisher, Emanuele Pesavento, Leslie Chasteen, Sara D’Angelo, Csaba Kiss, Michelle Longmire, Peter Pavlik, and Andrew R. Bradbury) overcame this obstacle by demonstrating a new method to display proteins that are normally expressed and folded in the cytoplasm. The team designed, created, and analyzed a large number of different vectors to display green fluorescent protein (GFP) on the phage surface. GFP is a protein that is normally expressed in the cytoplasm. By using GFP as the protein of interest, the team was able to identify when the protein had folded and displayed correctly: it would result in fluorescent phage. The best vector used a “twin arginine transporter” leader to transport the displayed protein to the site of phage assembly. In addition



to the display of other cytoplasmic proteins, this technology could enable the development of *fluorobodies*, or fluorescent antibodies, that were created by the team to facilitate target selection. The scientists are part of B-9’s Signature Ligand and Assay Development team and have been instrumental in developing multiple phage display technologies for use in ligand biochemistry. Some of these technologies have been licensed to pharmaceutical companies for use in applications such as drug development. Reference: “A Comprehensive Analysis of Filamentous Phage Display Vectors for Cytoplasmic Proteins: An Analysis with Different Fluorescent Proteins”, *Nucleic Acids Research* 2009 December 2 [Epub ahead of print]; doi: 10.1093/nar/gkp809. The DOE Genomes to Life Program and LANL Laboratory Research and Development supported the work.

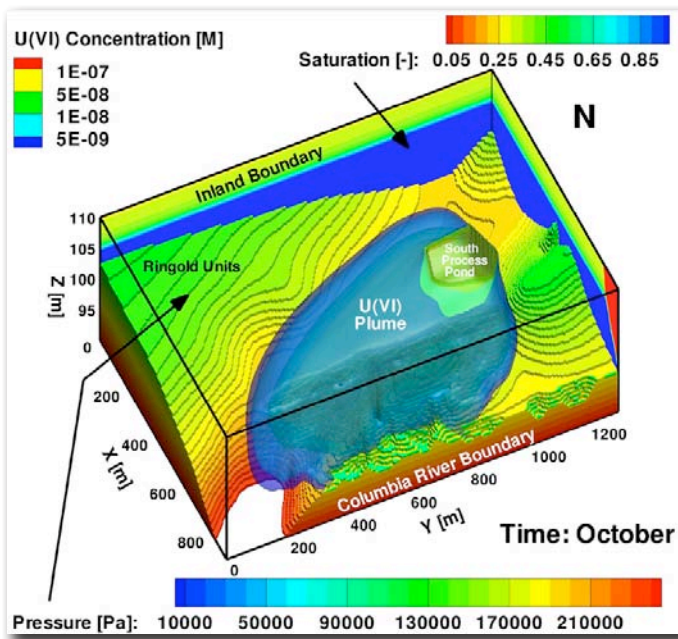
Figure 1. Structure of the green fluorescent protein.

## EARTH AND ENVIRONMENTAL SCIENCES

### **Ultrascale modeling of CO<sub>2</sub> sequestration and radionuclide migration**

The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program promotes cutting-edge research that can only be conducted with state-of-the-art supercomputers. The Leadership Computing Facilities (LCFs) at Argonne and Oak Ridge national laboratories, supported by the DOE Office of Scientific Computing Research, operate the program. The LCFs award sizeable allocations (typically tens of millions of processor hours per project) on powerful supercomputers to researchers from academia, government, and industry addressing grand challenges in science and engineering such as developing new energy solutions and gaining a better understanding of climate change resulting from energy use.

The INCITE program awarded Peter Lichtner (EES-16, Principal Investigator), Glenn Hammond (Pacific Northwest National Laboratory) and Richard Mills [Oak Ridge National Laboratory (ORNL)], 18,000,000 processor hours on ORNL’s XT Jaguar supercomputer. The project: “Ultrascale Simulation of Basin-Scale CO<sub>2</sub> Sequestration in Deep Geologic Formations and Radionuclide Migration Using PFLOTTRAN,” will investigate sequestration of greenhouse gases such as CO<sub>2</sub> in deep geologic formations to mitigate global warming, and migration of radionuclides from highly contaminated DOE legacy sites from World War II and the Cold War. By applying petascale computing to extreme-scale problems involving CO<sub>2</sub> sequestration in large geologic basins, the project will investigate the effects on drinking water aquifers of displacing deep formation water brines with large volumes of CO<sub>2</sub>. In addition, it will apply petascale resources to uranium migration at the Hanford 300 Area in Washington State along the Columbia River corridor. New data for stratigraphy, heterogeneity, and chemical



processes are becoming available as part of an ongoing DOE/Integrated Field Research Challenge (IFRC) project focused on the 300 Area. The INCITE project will incorporate this information into a larger revised site model. In addition, the project will assist members of the ORNL IFRC project in constructing a watershed-scale groundwater model with refined resolution using high performance computing for sites at the Oak Ridge Reservation. This model will integrate multiple processes at multiple scales into the model to investigate both the influence of process interactions at small scales on the fate and transport of contaminants in the field, and the scale dependency of controlling parameters such as dispersivity, attenuation, mass transfer, and reaction rates.

Figure 2. PFLOTTRAN simulation of uranium migration at the Hanford 300 Area in Washington State along the Columbia River corridor.

## LANSCE

### Understanding the pathogenesis of Alzheimer’s disease

Alzheimer’s disease is an irreversible, progressive brain disease that destroys memory and thinking skills, and eventually even the ability to carry out the simplest tasks. The brain develops abnormal clumps (amyloid plaques) and tangled bundles of fibers (neurofibrillary tangles) during the disease.

Amyloids are insoluble fibrous protein aggregates sharing specific structural traits. Abnormal accumulation of amyloid in organs may lead to amyloidosis, and may play a role in various other neurodegenerative diseases. One of the molecules which can form fibrous structures is the amyloid- $\beta$  (A $\beta$ ) peptide. Its misfolding and aggregation has been linked to the pathogenesis of Alzheimer’s disease. However, the driving forces and mechanism of A $\beta$  aggregation *in vivo* remain unresolved. A $\beta$  molecules are amphipathic. That means they contain both hydrophilic (water loving) and

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hydrophobic (water hating) regions, which make them highly surface active.

Jarek Majewski (LANSCE-LC) and collaborators (University of Chicago, University of New Mexico, University of Copenhagen, Gettysburg College, and Max-Planck Institute of Colloids and Interfaces), examined the effect of an idealized hydrophobic interface, the air/water interface, on the conformation, assembly state, and morphology of A $\beta$  peptides partitioned to the interface. It is important to study A $\beta$ 's interfacial dynamics at this interface to better understand the aggregation mechanism. The scientists used two surface-sensitive, complementary X-ray scattering techniques, grazing-incidence X-ray diffraction (GIXD) and X-ray reflectivity (XR), to resolve *in situ* angstrom-level details, and atomic force microscopy (AFM) to resolve micron-level organization of A $\beta$  adsorbed at the air/water interface. Incubation experiments evaluated the effect of surface adsorbed A $\beta$  to cause formation of fibrils.

Their research demonstrates that the A $\beta$  spontaneously adsorb to the air/subphase interface to form a contiguous, single molecular film about 20 angstroms thick. The film contains approximately 100 angstrom-sized ordered domains comprised of A $\beta$  peptides folded in a  $\beta$ -sheet conformation. Thus, when the otherwise unfolded A $\beta$  partitions to the interface, the peptide misfolds into a conformation found in amyloid fibrils. This conformation propagates over approximately 20 peptide molecules. This interface-driven misfolding and self-assembly of A $\beta$  is observed at nano-molar peptide concentrations, far below the concentration at which A $\beta$  aggregation occurs in bulk solution by homogeneous nucleation. The study shows that interface-adsorbed A $\beta$  can seed fibril formation (Figure 3). This result



indicates that interface-induced A $\beta$  folding and self-assembly may serve as a heterogeneous nucleation controlled aggregation mechanism by which A $\beta$  aggregates *in vivo*. Reference: “Amyloid- $\beta$  Fibrillogenesis Seeded by Interface-induced Peptide Misfolding and Self-assembly”, *Biophysical Journal* (in press). This work benefited from the use of the Lujan Neutron Scattering Center at LANSCE, which DOE’s Office of Basic Energy Sciences funds.

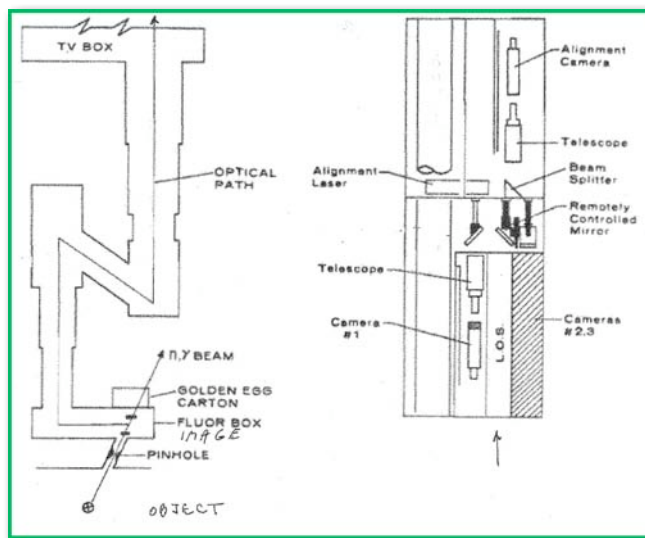
Figure 3. Transmission electron microscopy (TEM) image of 25  $\mu$ M A $\beta$  fibrils obtained after the surface-adsorbed A $\beta$  were re-introduced into the bulk and incubated for 5 days.

## PHYSICS

### New movie of Nevada Test Site shot

Scientists presented re-analysis of the FREEZEOUT Time-Resolved PINEX (TRP) at the Nuclear Explosive Device Physics Conference (NEDPC). TRPs are nearly unique in nuclear device diagnostics because they provide temporally and spatially resolved information on the neutron distributions. Similar to re-analysis of the COALORA TRP from 2007, the individual data frames were normalized to complementary NUEX (neutron experiment that measured the total number of neutrons coming up the line of sight vs. time) data. This provides an independent measure of the relative amplitude of each frame. Interpolation of the true data frames produced a movie representing nuclear processes within the device. The FREEZEOUT TRP differs from the COALORA TRP in its coverage across the nuclear process. Uncertainties were tracked through the image analysis process to enable quantitative validation of models for this particular device. Uncertainty analysis is particularly critical because TRPs pushed the





state of technology during testing. Chad Olinger (P-23) led the Nuclear Device and Data Science Team and the National Security Technologies Archiving Team. The Science Campaign Capability in Archiving Program and the Advanced Simulation and Computing Verification and Validation Program supported the work.

Figure 4. Generic line of sight design of a time resolved PINEX diagnostic fielded in a hole at Nevada Test Site; right side shows details in the T.V. (or PINEX camera) box.

## SCIENCE AND TECHNOLOGY BASE PROGRAM OFFICE

### LANL selects Distinguished Postdoctoral Fellows

Candidates for LANL Distinguished Postdoctoral Fellows display extraordinary ability in scientific research and show clear and definite promise of becoming outstanding leaders in the research they pursue. Up to two appointments are awarded from each category annually. Appointments are for three years. Sponsored candidates are reviewed by the Postdoctoral Committee annually at the January quarterly meeting. The *J. Robert Oppenheimer (JRO) Postdoctoral Fellowship* is named after the Laboratory's first Director. The fellowship provides the opportunity for recipients to collaborate with LANL scientists and engineers on staff initiated research. The JRO Fellowship is open to people of all nationalities. The *Richard P. Feynman (RPF) Postdoctoral Fellow in Theory and Computing* is named after the famed theoretical physicist and winner of the 1965 Nobel Prize in Physics. The fellowship provides the opportunity for recipients to collaborate with LANL scientists and engineers on staff-initiated research in the areas of theory and computing. The RFP Fellowship is restricted to U.S. citizens. The selected Fellows and their projects are described in the following paragraphs. All were currently at LANL as Director's Postdoc Fellows and now will move into their new appointment title.



**Shadi Dayeh:** As a Director's Postdoctoral Fellow, Dayeh (MPA-CINT) provided new insights into and control over the science of semiconductor nanowire growth at their ultimate size limit, and uniquely demonstrated novel growth techniques for 100 % doping and composition modulated Ge/Si axial and radial heterostructures. As an Oppenheimer Distinguished Postdoc Fellow, Dayeh plans to pursue semiconductor nanowire studies in a wide variety of areas, including electronics, spintronics, solar energy harvesting and electro-neural interface research. The title of his project is "Unique Semiconductor Nanowire Heterostructures in Physics and Applications". Tom Picraux (MPA-CINT) is his sponsor.

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**Alex Koglin:** As a Director's Postdoctoral Fellow, Koglin's (B-8) research has focused on developing methods for structure and dynamic elucidation of very large membrane associated proteins focused on antibiotic and siderophore biosynthetic clusters and resistance. The thrust of his research as an Oppenheimer Distinguished Postdoc Fellow will be analyzing protein structures and the function relations in antibiotic biosynthesis and signal transducing receptors by NMR spectroscopy. The title of his project is "Analysis of Protein Structure and Function Relations in Antibiotic Biosynthesis and Signal Transducing Receptors". This is a LANL and Harvard Medical School collaboration. Pete Silks (B-8) sponsors Koglin.



**Brian Munsky:** During his PhD research, Munsky (CCS-3/B-9) developed the Finite State Projection method, a unique computational approach that has blossomed into a subfield of research in analysis of stochastic systems and his research as a Director's Postdoctoral Fellow has built on this approach and used it to identify and validate predictive stochastic models for gene regulation in bacteria and yeast. For his Feynman Distinguished Postdoc Fellow appointment, he will partner with LANL's National Flow Cytometry Resource to identify stochastic models of cellular regulation, and to improve design of experiments involving single-cell assays of cellular behavior. The title of his project is "Quantitative Models of Cellular Noise". Michael Wall (CCS-3) and Babs Marrone (B-9) co-sponsor Munsky.



**Adrian Pope:** As a Feynman Distinguished Postdoc Fellow, Pope's (ISR-1/T-2/CCS-6) research is aimed at understanding the formation of structure in the Universe. The distribution of galaxies holds essential clues regarding properties of dark energy and dark matter. In order to get at the exciting foundational science, his work encompasses observations, theory, computation, and statistics. He has carried out major work on the Sloan Digital Sky Survey and recently played a key role in "Roadrunner Universe" – one of the recent open science projects run on LANL's Roadrunner supercomputer. The title of his project as a Feynman Distinguished Postdoc Fellow is "Tracing Fluctuations in the Universe". Katrin Heitmann (ISR-1), Salman Habib (T-2), and Dave Higdon (CCS-6) sponsor Pope.

## THEORETICAL

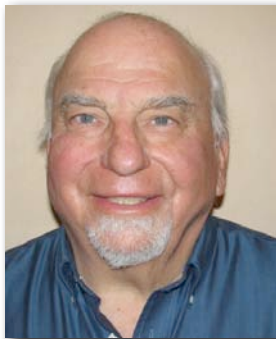
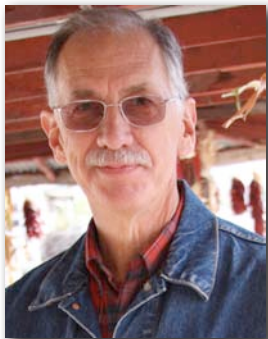
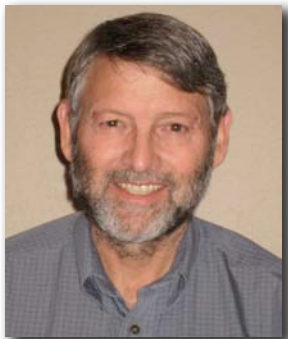
### American Physical Society recognizes outstanding referees Albers, Finn, Ginocchio, Sierk



The American Physical Society (APS) selected LANL scientists Robert C. Albers, John M. Finn, Joseph N. Ginocchio, and Arnold J. Sierk as Outstanding Referees. The Outstanding Referee Program recognizes scientists who have been exceptionally helpful in assessing manuscripts for publication in the APS journals. The Editors select the honorees based on the quality, number, and timeliness of their reports, without regard for membership in the APS, country of origin, or field of research. Referees are rewarded for their work carried out since 1978, the earliest year for which we have accurate data on referee reports returned. By means of the program, APS expresses its appreciation to all referees, whose efforts in peer

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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. The highly selective Outstanding Referee program annually recognizes about 150 of the roughly 45,000 currently active referees. Like Fellowship in the APS, this is a lifetime award.



Photos (left to right): Robert C. Albers, John M. Finn, Joseph N. Ginocchio, and Arnold J. Sierk