# ALS SPECTRUM

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What's Inside:



U.S. DEPARTMENT OF ENERGY
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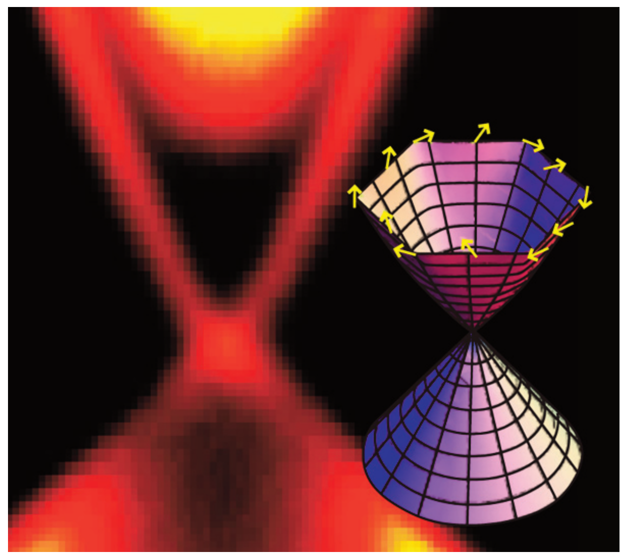
ALS ADVANCED LIGHT SOURCE

ALS COMMUNICATIONS

## ALS Reveals New State of Matter

ALS user groups from Princeton and Stanford have been making waves this past year with several high-profile papers and extensive news coverage of their work on a new state of matter embodied by so-called "topological insulators," materials that conduct electricity only on their surfaces. First identified at the ALS in 2007 by a Princeton team led by M. Zahid Hasan, topological insulators have been the subject of intense interest, based on unusual quantum properties that manifest themselves macroscopically. The discovery of a "second generation" of topological insulators that robustly retain these properties well above room temperature has spurred a rising tide of theoretical proposals for potential applications in nanoscale spintronic devices and fault-tolerant quantum computers. In addition, it's also been suggested that topological insulators may serve as a test bed for studies of never-before-seen particles predicted by high-energy physics.



Band structure of the topological insulator, bismuth selenide ($Bi_2Se_3$). The red areas represent surface states. The vertical space between the yellow areas is the bulk band gap (about 0.3 eV). Because the surface states cross the band gap, this "insulator" conducts electricity on its surface. Inset: Three-dimensional schematic of the cone-shaped surface band structure. The spin states (yellow arrows) indicate that electrons on the surface won't backscatter from disorder and impurities. (Image courtesy of David Hsieh, Yuqi Xia, and Andrew Wray, Princeton University).

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## User Support Building Opens for Business

The ALS User Support Building (USB), a facility whose need was identified in the first days of ALS operations, is now complete and open for use. The $35 million project faced many funding challenges over the years, but with the American Recovery and Reinvestment Act providing the final $14.5 million needed a year ahead of schedule, the project was able to proceed ahead of plan.

The 30,000 square foot building provides users and staff over 4000 square feet of badly needed experimental staging area with all the requisite utilities, a high bay, and a two-ton-capacity bridge crane. The staging

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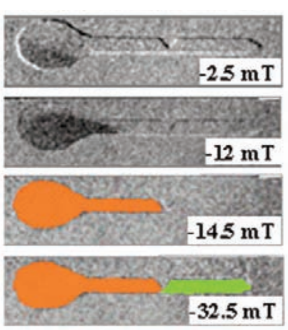
# Science Roundup

### Stochastic Domain-Wall Depinning in Magnetic Nanowires

Im et al., *Nature* **459**, 820 (2009)

Reliably controlling the motion of magnetic domain walls along magnetic nanowires is a key requirement for current technological development of novel classes of logic and storage devices, but understanding the nature of nondeterministic domain-wall motion remains a scientific challenge. A statistical analysis of high-resolution magnetic soft x-ray microscopy images by a Berkeley Lab–University of Hamburg group has now revealed that the stochastic behavior of the domain-wall depinning field in notch-patterned $Ni_{80}Fe_{20}$ (permalloy) nanowires depends strongly on the wire width and the notch depth. This result both provides valuable insight into the motion of magnetic-domain walls and opens a path to further technological developments in spintronics applications.

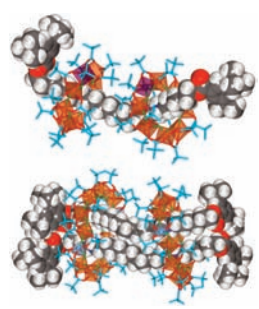



Domain-wall evolution patterns. Analysis of 40 measurements for wires with different widths and notch depths demonstrates that domain-wall motion depends on the width and depth, thereby providing a path to minimizing this behavior.

### Hybrid Rotaxanes: Interlocked Structures for Quantum Computing?

Lee et al., *Nature* **458**, 314 (2009)

Rotaxanes are mechanically interlocked molecular architectures consisting of a dumbbell-shaped molecule, the "axle," that threads through a ring called a macrocycle. Because the rings can spin around and slide along the axle, rotaxanes are promising components of molecular machines. While most rotaxanes have been entirely organic, the physical properties desirable in molecular machines are mostly found in inorganic compounds. Working together, two British groups at the University of Edinburgh and the University of Manchester have bridged this gap with hybrid rotaxanes, in which inorganic rings encircle the organic axles. The hybrid architecture greatly increases their range of useful physical properties, such as the magnetism based on molecular magnets that may make them suitable as qubits for quantum computers.

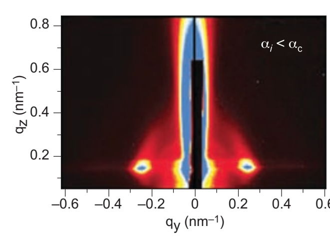


The structures of the [3]- and [4]rotaxanes as determined by x-ray single-crystal diffraction. The organic threads are shown as space-filling spheres (hydrogen, white; carbon, grey; oxygen, red; and nitrogen, blue) and the inorganic rings as a mixture of polyhedra (chromium, orange; cobalt, purple; and copper, blue) and stick representations (carbon, blue; oxygen, red; and fluorine, green).

### Proton Channel Orientation in Block-Copolymer Electrolyte Membranes

Park et al., *Adv. Mater.* **21**, 203 (2009)

Fuel cells have the potential to provide power for a wide variety of applications ranging from electronic devices to transportation vehicles. Cells operating with $H_2$ and air as inputs and electric power and water as the only outputs are of particular interest because of their ability to produce power without degrading the environment. Polymer electrolyte membranes (PEMs), with hydrophilic, proton-conducting channels embedded in a structurally sound hydrophobic matrix, play a central role in the operation of polymer electrolyte fuel cells. PEMs are humidified by contact with air (the presence of water in PEMs is essential for proton transport). In addition, PEMs must transport protons to catalyst sites, which are typically crystalline solids such as platinum. The arrangement of the hydrophilic domains in the vicinity of both air and solid substrates is thus crucial. Researchers have now provided the first set of data on the morphology of PEMs at interfaces by a combination of x-ray scattering and microscopy.

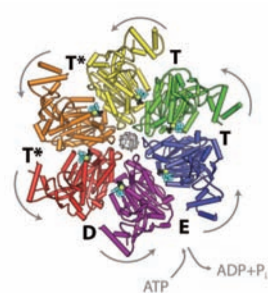



A PEM scattering pattern dominated by contributions from the PEM surface shows well-defined spots, indicating the presence of hydrophilic channels oriented perpendicular to the surface, ideal for water transport. In contrast, scattering patterns from the bulk PEM exhibited a scattering ring, indicating the presence of hydrophilic channels parallel to the plane of the film.

### Rotary Firing in Ring-Shaped Protein Explains Unidirectionality

Thomsen et al., *Cell* **139**, 523 (2009)

Hexameric motor proteins represent a complex class of molecular machines that variously push and pull on biological molecules using adenosine triphosphate (ATP) as chemical fuel. A specialized class of ring-shaped motor proteins, hexameric helicases, can unwind DNA strands and perform large-scale manipulations of single-stranded nucleic acids in processes such as DNA replication, DNA repair, and gene expression. To understand how certain hexameric helicases walk with directional polarity along single-stranded nucleic acids, Berkeley researchers used x-ray crystallography at the ALS




The structure of the hexameric Rho transcription termination factor. The positions of the subunits (E, T, T*, and D) dictate the direction of the ATPase cycle (arrows). This mechanism is analogous to the firing order of cylinders in an internal combustion engine; reversing the order of the subunits reverses the direction of "crankshaft" rotation.

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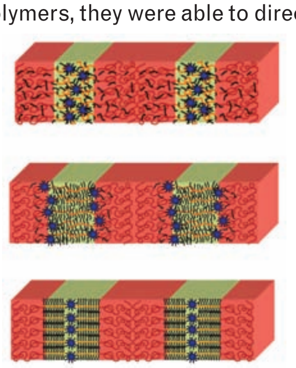
*Read more about these and other science highlights at http://www.als.lbl.gov/index.php/science-highlights/science-highlights.html.*

to solve the structure of a hexameric helicase, the Rho transcription termination factor (from *E. coli*), bound to both ATP mimics and an RNA substrate. The results showed that Rho functions like a rotary engine: as the motor spins, it pulls RNA strands through it's interior. Interestingly, the rotary firing order of the motor is biased so that the Rho protein can walk in only one direction along the RNA chain.

### A New Route to Nano Self-Assembly

Zhao et al., *Nat. Mater.* **8**, 979 (2009)

If the promise of nanotechnology is to be fulfilled, nanoparticles will have to be able to make something of themselves. An important advance toward this goal has been achieved by researchers who have found a simple and yet powerfully robust way to induce nanoparticles to assemble themselves into complex arrays. By adding specific types of small molecules to mixtures of nanoparticles and polymers, they were able to direct the self-assembly of the nanoparticles into arrays of one, two, and even three dimensions with no chemical modification of either the nanoparticles or the block copolymers. In addition, the application of external stimuli, such as light and/or heat, can be used to further direct the assemblies of nanoparticles for even finer and more complex structural details, a result verified by small-angle x-ray scattering (SAXS) at the ALS.

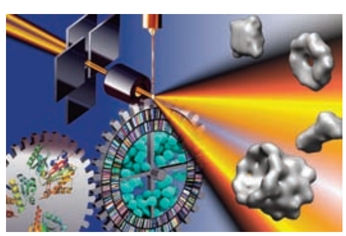


Schematics depicting how the nanoparticles were rearranged during heating and cooling: the nanoparticles (blue) assembled in the center of mediating layers (tan) from 50 to 100°C (bottom), at the interfaces between the layers at 110°C (middle), and were randomly distributed in the layers at 150°C (top).

### Robust, High-Throughput Analysis of Protein Structures

Hura et al., *Nat. Methods* **6**, 606 (2009)

Scientists have developed a fast and efficient way to determine the structure of proteins, shortening a process that often takes years into a matter of days. The Structurally Integrated BiologY for Life Sciences (SIBYLS) beamline at the ALS has implemented the world's highest-throughput biological-solution x-ray scattering beamline enabling genomic-scale protein-structure characterization. Coupling brilliant x rays from one of the superconducting bend magnets at the ALS to liquid-handling robotics has enabled the collection of 96 samples in 4 hours. Importantly, the sample format and the amount of material required are practical for most biological problems. The beamline's high-throughput capability is set to have a large impact on many fields that require genomic-scale information, such as Berkeley Lab's bioenergy efforts and cancer biology studies.

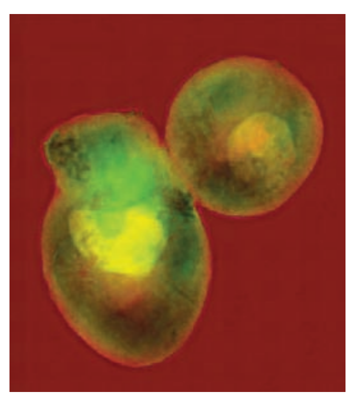


Artist's abstract depiction of high-throughput SAXS combining high-brightness x rays, robotic handling, and computation as applied to all the gene products (i.e., proteins) of a microorganism, resulting in the shape and assembly of each macromolecule.

### Lensless Imaging of Whole Biological Cells with Soft X Rays

Nelson et al., *PNAS* **107**, 16 (2010)

A team of scientists has used x-ray diffraction microscopy at ALS Beamline 9.0.1 to make images of whole yeast cells, achieving the highest resolution—11 to 13 nanometers (billionths of a meter)—ever obtained with this method for biological specimens. Their success indicates that full 3-D tomography of whole cells at equivalent resolution should soon be possible. Large numbers of cells can currently be processed in a short time at resolutions of 40 to 60 nanometers, but the ability to increase resolution to the 10-nanometer range would enhance research capabilities in both biology and materials sciences.

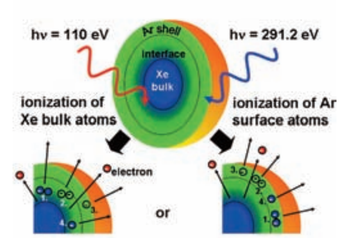


A pair of yeast cells imaged at very high resolution using coherent soft x rays. The coherent (laser-like) beam of penetrating x rays allows a computer to reconstruct the cells' internal structures from a diffraction pattern, without focusing the light with a lens.

### Site-Selective Ionization in Nanoclusters Affects Subsequent Fragmentation

Hoener et al., *Phys. Rev. A* **81**, 021201(R) (2010)

Understanding charge-transfer processes at the atomic level of nanoscale systems is of the utmost importance for designing nanodevices based on quantum-dot structures, nanotubes, or two-dimensional graphene sheets. Researchers from Western Michigan University, Berkeley Lab, and other international research facilities investigated charge-transfer processes and subsequent ion fragmentation dynamics in nanoclusters composed of argon (Ar)




The different photoionization cross-sections of Xe 4d and Ar 2p electrons enable site-selective ionization of the cluster's bulk (Xe) or surface (Ar). By measuring coincidences between the subsequent photoelectrons and the resulting ionic cluster fragments, charge-transfer and fragmentation processes can be determined.

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## A New State of Matter

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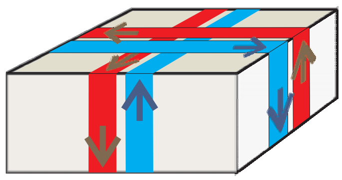
The research from Princeton and Stanford (Yulin Chen and others from Z.-X. Shen's group) used angle-resolved photoemission spectroscopy (ARPES) to identify new classes of topological insulator materials and to establish key traits of their unique electronic environment. The Princeton group worked at ALS Beamlines 12.0.1 and 10.0.1 as well as Stanford Synchrotron Radiation Lightsource (SSRL) Beamline 5-4, while the Stanford group worked at ALS Beamline 10.0.1 and SSRL Beamline 5-4. Their results have reinforced the importance of synchrotron light sources as an indispensable tool in exploring matter in the twenty-first century.

The experimental results show that electrons in topological insulators are constrained by a very different set of rules than are electrons in normal matter. Macroscopic topological insulators are referred to as insulators because electrical conductivity is very weak deep inside the bulk of the crystal; however, a skin of highly conducting states becomes available as electrons draw close to the crystal surface, making the physical system of a topological insulator crystal analogous to a hollow metallic box. The photoemission measurements confirmed that these surface states are described in momentum space by an odd number of Dirac cones, which signify electrons that behave as if they have no mass. In addition, the spin-sensitive measurements showed that



Schematic of the two-dimensional surface states in a three-dimensional topological insulator. The red and blue strips represent surface currents with opposite spin character.

the surface conduction states are spin polarized: electrons with a given spin will all move in the same direction along the surface and retain their quantum phase.

The researchers combined atomic-scale scanning tunneling microscopy and spin-resolved photoemission measurements to show that the nature of spin polarization in topological insulators removes the ability of electrons to backscatter (no "U-turns" for electrons) and largely protects them from all scattering that would be caused by impurities and defects in a normal conducting material. Scattering from defects is a source of electrical resistance, wavefunction decoherence, and electron localization, all of which are obstacles to device engineering with normal materials on the nanometer scale. This opens the door to many advances in spintronics and quantum computing.

The Princeton collaboration originally identified a bismuth antimony alloy ($Bi_{1-x}Sb_x$) to be the first known three-dimensional topological insulator in

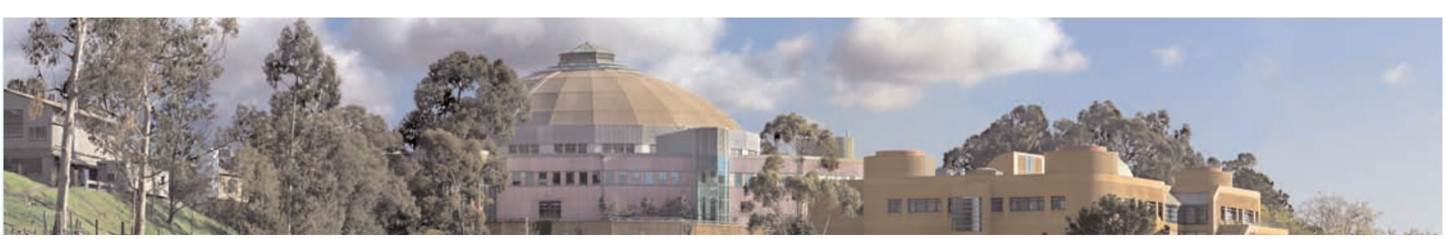
Three-dimensional image of the surface band structure of bismuth telluride ($Bi_2Te_3$). The V-shaped pure surface state is nearly isotropic in the momentum plane, forming a Dirac cone in momentum space. (Image courtesy of Yulin Chen and Z.-X. Shen, Stanford University.)

2007 and hypothesized that a closely related class of bismuth-based material, the bismuth selenide ($Bi_2Se_3$) class, should also display similar topological behavior but with a larger bulk insulating gap, simpler Dirac electron kinetics, and possibly much higher operating temperatures. Investigations by Princeton, Stanford, and several other groups throughout 2009 have confirmed that a significant class of materials with the chemical formula $M_2X_3$ (M = Sb, Bi; X = Se, Te) can achieve topological behavior (in most cases), and the bulk band gap in $Bi_2Se_3$ in particular was seen in photoemission experiments to be the largest (around 300 meV), setting an energy scale record that renders the topological insulator state stable up to the crystalline melting point (~710 °C, or 1310 °F).

Beyond their potential for practical applications, topological insulators may also provide a way to study fundamental particle physics—a "tabletop universe" of sorts. Some researchers believe that the conditions inside this new state of matter can be manipulated (for example, by bringing it into contact with a superconductor or adding an electromagnetic field) in ways that cause electrons to simulate the quantum properties of theorized but elusive particles. Examples of such exotic particles include axions (a possible constituent of dark matter), magnetic monopoles (poles of north and south magnetism isolated from each other), and Majorana particles (fermions that function as their own antiparticles).

The successful collaborative application of diverse experimental techniques confirms that the spectroscopic tools for identifying and investigating the physics of still more topological insulator materials are developing rapidly. Taken collectively, the latest results have already uncovered an exciting macroscopic quantum environment, in which new physical rules create a new realm of phenomenological possibilities.

Publications about this work: D. Hsieh et al., *Nature* **452**, 970 (2008); D. Hsieh et al., *Science* **323**, 919 (2009); Y. Xia et al., *Nat. Phys.* **5**, 398 (2009); Y.L. Chen et al., *Science* **325**, 178 (2009); D. Hsieh, *Nature* **460**, 1101 (2009); P. Roushan et. al., *Nature* **460**, 1106 (2009); and D. Hsieh et al., *Phys. Rev. Lett.* **103**, 146401 (2009). ■



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# Experimental Systems Group: Focus on Brightness

by Howard Padmore

The ALS has developed over the years a complementary portfolio of infrared, VUV, soft x-ray, medium-energy, and hard x-ray beamlines. The hard x-ray techniques are focused on the DOE's energy mission—advancing our understanding, for example, of polymer chemistry and physics related to plastic electronics and solar cells, interfaces in batteries, the properties of new lightweight composite materials, and the structure of new catalysts. In the lifecycle of a beamline, there is a long stretch of time after initial operation in which performance can be steadily improved, often by orders of magnitude, by use of new technologies. Here we report on a few of these developments that are emblematic of the advances that are constantly made.

## Diffractive Imaging and COSMIC

The redevelopment of Sector 7.0 is the next item to be implemented as part of the ALS strategic plan. Funding has been obtained for this, to build MAESTRO for nanoARPES and COSMIC for coherent imaging. The design permits COSMIC scattering to be added to the beamline as funding allows. COSMIC will build on the enhanced brightness of the ALS post–top-off with a pair of special beamlines designed to provide modest spectral resolution as well as to preserve the source brightness and stability and match the photon phase-space into the illumination requirements for coherence experiments. We designed the beamline facility in 2007 and we will implement it over the next couple of years. The first instrument being developed for COSMIC as part of an LDRD project is called the Nanosurveyor. It will emphasize tomography with high-resolution ptychography [H.N. Chapman, *Science* **321**, 352 (2008)], a technique now made possible at these wavelengths thanks to fast detectors developed at Berkeley Lab [P. Denes et al., *Rev. Sci. Instrum.* **80**, 083302 (2009)]. The aim of the Nanosurveyor is to provide selected area diffraction; spectroscopy and imaging at close to diffraction-limit resolution; and the ability to navigate, zoom in, and collect tomographic data sets or large-area surveys of a sample.

## Ultrahigh-Resolution Grating Optics

To exploit the potential of high-resolution resonant inelastic soft x-ray spectroscopy (RIXS), a resolving power of $10^5$—$10^6$ is required over the energy range from 0.5—1.0 keV. This is 100 times better than currently available. Moreover, due to the small Raman x-ray cross section, a useful spectrometer has to be highly efficient. This performance cannot be obtained with conventional grating optics because (1) slit sizes would be extremely small and almost all flux would be lost; (2) extremely large spectrometers would be required; and (3) because of (1) and (2), unrealistically small optical slope errors would be required of the optics of the emission spectrometer.

We are developing a technology to fabricate the efficient diffraction gratings with high dispersion that are needed to solve these problems. These are high-density diffraction volume x-ray gratings, consisting of a multilayer coating deposited on an echellette substrate. Such a grating can diffract with very high efficiency in high diffracted orders if diffraction conditions for in-plane (grating) and out of plane (Bragg multilayer) are met simultaneously. A fabricated prototype grating optimized for diffracting in the third order (an effective groove density of 15,000 lines/mm) at a

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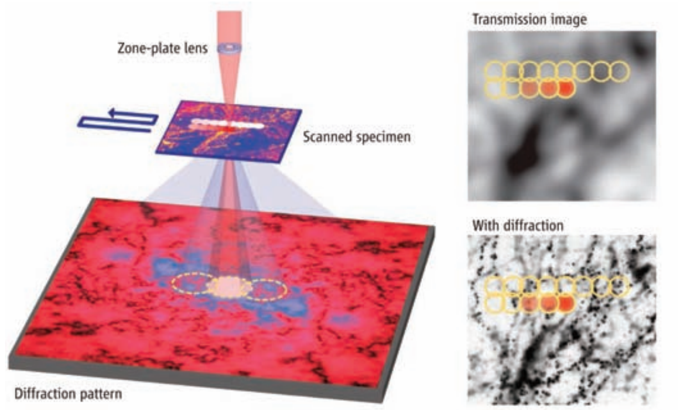
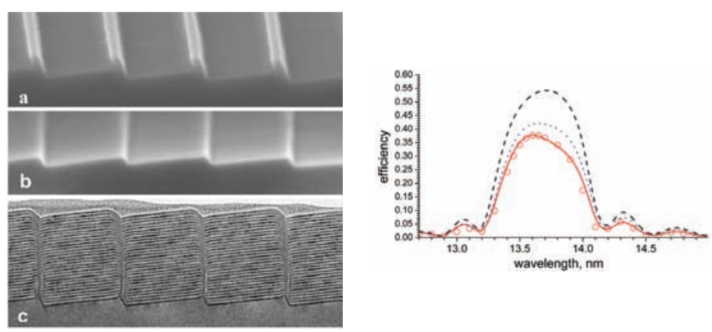



Left (from Chapman et al.): In soft x-ray ptychography, a zone plate is used to focus an x-ray beam onto a slab of sample. Transmission diffraction patterns are rapidly read out for many positions of the probe as it is scanned across the sample. By collecting and analyzing entire diffraction patterns at each probe position, ptychography can provide phase-contrast images with much higher resolution than that of the probe-forming lens.




Left: SEM images of a 200-nm echellette grating (a) after KOH etch and nitride mask removal, (b) after nub removal, and (c) cross-section TEM image of the grating coated with the Mo/Si multilayer. Right: Measured (circles) and simulated (lines) efficiency of the third-order diffraction. The simulation was performed for an ideal groove profile (dashed curve) and for the measured profile before (dotted curve) and after (solid curve) deposition of the Mo/Si-30 multilayer.

## Experimental Systems Group

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wavelength of 13.6 nm has been demonstrated to provide an unprecedented efficiency of 37.6% [D.L. Voronov et al., *Opt. Lett.* **35**, 2615 (2010)].

As part of an LDRD project we are working on fabrication of similar gratings for the soft x-ray energy range and on their application in a superhigh-resolution EUV spectrometer. Due to the unique properties of the gratings, it is possible to design a spectrometer with a total length of only a few meters. For comparison, at 940 eV, a spectrometer using a conventional Au-coated blazed grating would be 11.2 m long and require a very long (500-mm) grating to achieve the same angular acceptance, with a very tight rms slope error tolerance of 70 nanoradians [D.L. Voronov et al., *AIP Conf. Proc.* **1234**, 776 (2010)].

As the source brightness improves, it creates a greater need to improve beamline optics, using the types of automated methodologies described above. It also puts a greater emphasis on using the best detector technologies available, such as commercial pixel detectors, and on new in-house-designed, energy-sensitive x-ray CCDs. Like the storage ring, which over the last 15 years has improved in brightness by a factor of 100, similar or even larger gains can be made with relatively modest investments in beamlines and endstations. With these improvements, we can look forward to a bright future! ■

## Scientific Support Group: New Beamlines, Great Science

by Zahid Hussain, Mike Martin, and Eli Rotenberg

**New Infrared Beamline 5.4.** The new infrared Beamline 5.4, dedicated to environmental, biological, and ultrahigh-resolution studies with mid- and far-infrared light, had its ribbon-cutting ceremony this year. The beamline and endstations are being commissioned and users are anticipated during the January–June 2011 cycle. The new beamline will collect double the light of the existing IR beamline and is expected to have endstations including complementary analytical capabilities. The endstations are uniquely located on top of the linac/beam test facilty cave inside the storage ring. This novel location allows additional space for clean biology sample preparations, which will facilitate many environmental and biological science needs when studying living systems.

**AMBER Proposal and Beamline 8.0 Plans.** AMBER, the Advanced Materials Beamline for Energy Research, is the new facility planned to replace the existing resonant inelastic soft x-ray scattering branchline at Beamlines 7.0.1 and 8.0.1. It comprises a coordinated pair of branchlines and endstations and features a new dedicated "half" insertion device capable of full polarization control along with higher flux and better energy resolution. The beamline will be based on a modern design concept that uses a variable-included-angle and variable-line-space grating monochromator. Both endstations provide substantially upgraded capabilities to our existing facilities. The new beamline is especially optimized for challenging experiments in the 50- to 2500-eV energy range, for measurements of the electronic structure of energy-related materials in a real-world environment. The beamline is optimized for in-situ photon-in/photon-out soft x-ray spectroscopy (PIPOS) and ambient-pressure x-ray photoemission spectroscopy (APXPS) and will be available to the leading research groups in the field of renewable energy science.

Mike Martin (Scientific Support Group Deputy for Operations) welcomes guests to the dedication ceremony for Beamline 5.4 and the Berkeley Synchrotron Infrared Structural Biology (BSISB) program.


Ribbon-cutting at Beamline 5.4 (L to R): Paul Alivisatos (Berkeley Lab Director), Hoi-Ying Holman (Earth Sciences Division), Bob Schoenlein (ALS Deputy Division Director for Science), Mina Bissell (Life Sciences Division), Ernie Majer (Earth Sciences Division), and Roland Hirsch (DOE). See *http://www.lbl.gov/publicinfo/newscenter/tabl/2010/march/03-24-10/jump.html* for more.

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## RING AROUND THE RING AROUND THE RING AROUND THE RING AROUND THE RING AROUND THE RING

**MAESTRO Construction Update.** A conceptual design review (CDR) was held for the nanoARPES endstation mechanical aspects on June 11. The meeting was attended by a number of engineering and scientific staff. Talks were presented by A. Bostwick and G.A. Gaines on the goals of the endstation design, and a conceptual design intended to meet those goals, pursuant to more detailed design. Verbal and written comments have been collected and a report on the CDR outcome was filed in July.

**MAESTRO Recent Science.** A team led by Aaron Bostwick and Eli Rotenberg in collaboration with groups in Germany, Italy, Iran, and Texas have published a paper: "Observation of Plasmarons in Quasi-Freestanding Doped Graphene," *Science* **328**, 999 (21 May 2010). The discovery demonstrates the possible suitability of graphene for use in plasmonic devices, which merge electronic and photonic technologies. Photons are known to couple to plasmons, and this work shows that plasmons strongly couple to electrons. Thus, indirect photon–electron coupling is suggested by the work. Shortly after publication, a Wikipedia article, "Plasmaron," appeared that succinctly defines what a plasmaron is: "In physics, a plasmaron is a quasiparticle arising in a system that has strong plasmon–electron interactions. It is a quasiparticle formed by quasiparticle–quasiparticle interactions, since both plasmons and electron holes are collective modes of different kinds. It has recently been observed in graphene and earlier in elemental bismuth." The news was covered in a Berkeley Lab press release: *http://newscenter.lbl.gov/news-releases/2010/05/20/plasmonic-promises/*.

**Effect of Strain on Electronic Properties.** The difference in lattice constant of a substrate compared to a thin film deposited on it or of a matrix compared to a nanocolumn induces a lattice distortion—i.e. strain—in the nanostructure as compared to the bulk. As a result, the properties of thin films and nanocolumns can be tuned to be markedly different than the intrinsic properties of the corresponding unstrained bulk materials. A research team at Beamline 4.0.2 has shown that soft x-ray absorption techniques are uniquely suited to provide detailed information on the impact of strain on the electronic properties of magnetic oxide nano-architectures in an element-, valence-, and site-specific way. Using an eight-pole electromagnet, they observed for the first time a strong dependence of the x-ray magnetic circular dichroism (XMCD) spectral shape on the experimental geometry of $MnCr_2O_4$ thin films that, in turn, is sensitive to the film strain state. This angle-dependent XMCD is a general phenomenon that will occur in any strained magnetic transition-metal oxide, creating for the first time the opportunity to study strain using soft x-ray spectroscopy and microscopy techniques on ultrafast time scales with nanometer spatial resolution. A superconducting eight-pole magnet providing magnetic fields of up to 6 T in arbitrary directions has recently been funded with $1.5 M through the American Recovery and Reinvestment Act and is under development to extend the XMCD capabilities to higher fields for experiments on a wide variety of complex oxides, dilute magnetic semiconductors, and engineered magnetic nanostructures.

**New Science.** These selected highlights from the past year reflect not only world-class science but illustrate the unique capabilities represented by the ALS Scientific Support Group (SSG).

- Biomimetic Dye Molecules for Solar Cells, *J. Chem. Phys.* **131**, 194701 (2009). *http://ssg.als.lbl.gov/highlights/12-envsci/130-biomimetic-dye-molecules-for-solar-cells*
- Electron Correlation in Iron-Based Superconductors, *Phys. Rev. B* **80**, 014508 (2009). *http://ssg.als.lbl.gov/highlights/18-semiconduct/126-electron-correlation-in-iron-based-superconductors*
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- Viewpoint: The all-organic route to doping graphene, *Physics* **3**, 46 (2010). *http://physics.aps.org/articles/v3/46*

**Mentoring and Pipeline for Future Scientists.** Establishing a pipeline for future beamline and accelerator scientists is vital to all DOE Basic Energy Science user facilities. Many SSG members mentor students at all levels throughout the year. The SSG has also established the ALS as leader in setting up the pipeline for synchrotron scientists by establishing graduate-student and postdoctoral fellowship support programs. *http://www.als.lbl. gov/als/fellowships/* ■

## Chemical Dynamics: Electronic Structure of the Building Blocks of Life

by Musa Ahmed

The molecular structures of many biological molecules are well known, in light of the 57 years of research that have elapsed since Watson and Crick's original postulation for the structure of DNA. However, fundamental aspects, such as the electronic structure of these building blocks of life, are not yet well understood. The ionization of DNA bases is a key initial step that leads to DNA damage and mutation. The electron hole that is introduced by the ionization process migrates along the DNA's helix through various hopping mechanisms, leading to tautomerization through proton transfer and dissociation in the strand of the helix itself. Apart from the evolutionary and carcinogenic effects this damage might induce in living systems, there is also

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## Chemical Dynamics

continued from page 7

much interest in the electronic properties of the DNA molecules themselves for use in molecular electronics.

At the Chemical Dynamics Beamline (9.0.2), we have initiated a rigorous program to prepare DNA bases [Zhou et al., J. *Phys. Chem. A* **113**, 4829 (2009); Zhou et al., *Anal. Chem.* **82**, 3905 (2010)] and their dimers [Bravaya et al., *PCCP* **12**, 2292 (2010); Kostko et al., *PCCP* **12**, 2860 (2010)] in the gas phase, by thermal and laser desorption and ion-beam sputtering, with subsequent interrogation via single-photon ionization using tunable VUV light. The resulting measurements allow unique insight into the electronic structure of these systems when compared to state-of-the-art theory being performed by Anna Krylov's group at the University of Southern California as well as in-house. The photoionization dynamics of gas-phase adenine–adenine (AA), thymine–thymine (TT), adenine–thymine (AT), cytosine–cytosine (CC), guanine–guanine (GG), and guanine–cytosine (GC) dimers was investigated, yielding the first experimental measurements of the ionization energies of these dimers. An unprecedented insight into the effect of noncovalent interactions (i.e., hydrogen bonding, stacking, and electrostatic interactions) on the ionization energies of the individual nucleobases was obtained. The origin of this effect and the character of the ionized states are different in asymmetric H-bonded and symmetric stacked isomers. The ionization of the H-bonded dimers results in barrierless (or nearly barrierless) proton transfer, whereas the π-stacked dimers relax to structures with the hole stabilized by the delocalization or electrostatic interactions. Both experimental and theoretical results suggest that a number of tautomers and H-bonded dimers are present in the molecular beam; however, a more quantitative analysis would require calculations of Frank Condon factors and ionization cross sections, which are underway. Furthermore, by comparing the

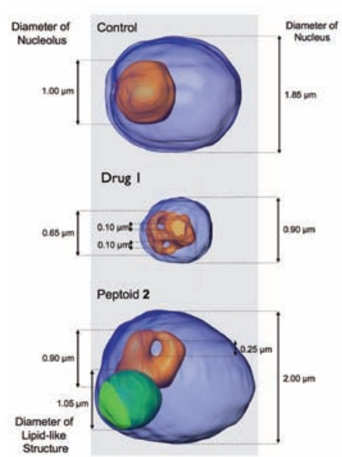
Cover art for PCCP **12**, 2292 (2010) depicting π-stacking and H-bonding interaction motifs in DNA. Courtesy of Vadim Mozhayskiy (USC).

fragmentation patterns of thymine generated via ion sputtering vs thermal desorption (Zhou et al., 2009) and of guanine generated in laser vs thermal desorption (Zhou et al., 2010) the nature of internal energies in desorption processes was elucidated. ■

## NCXT: Imaging Pathogenic Yeast Cells

by Gerry McDermott

The National Center for X-Ray Tomography (NCXT) soft x-ray microscope, XM-2, is about to complete its first year of operation as a user beamline. Even so, demand for access to this beamline has been very high and continues to grow. Since it opened for business, the beamline has already been used by research groups from as far afield as Korea, England, and Australia. To date, users have collected several thousand tomographic data sets, from specimens that range in size from small, simple bacteria to large eukaryotic cells. For example, Annalise Barron and Modi Wetzler from Stanford University worked with the NCXT team to determine how peptoids—a promising new line of antimicrobial drugs—prevent pathogenic yeast from causing disease. In particular, they were interested in studying the effect of these candidate drug molecules on the yeast *Candida albicans.* Most people are unaware they have this yeast living on their skin or in their intestines. However, under certain conditions—for example, after taking a course of antibiotics—this yeast can undergo a phenotypic transition, similar to Dr. Jekyll becoming Mr. Hyde. When this happens, the yeast becomes pathogenic and can cause disease. In most instances, this is a relatively minor, albeit uncomfortable condition that can be easily treated with antifungal drugs. But in instances where the yeast has become resistant to existing antifungal drugs or the infection has become systemic, the condition is serious and frequently life threatening. The Barron group has developed peptoids specifically aimed at stopping the yeast




The effect of peptoid treatment on the nucleus of *Candida albicans.*


G. McDermott, M.A. Le Gros, C.G. Knoechel, M. Uchida, and C.A. Larabell, *Trends Cell Biol.* **19**, 587 (2009).

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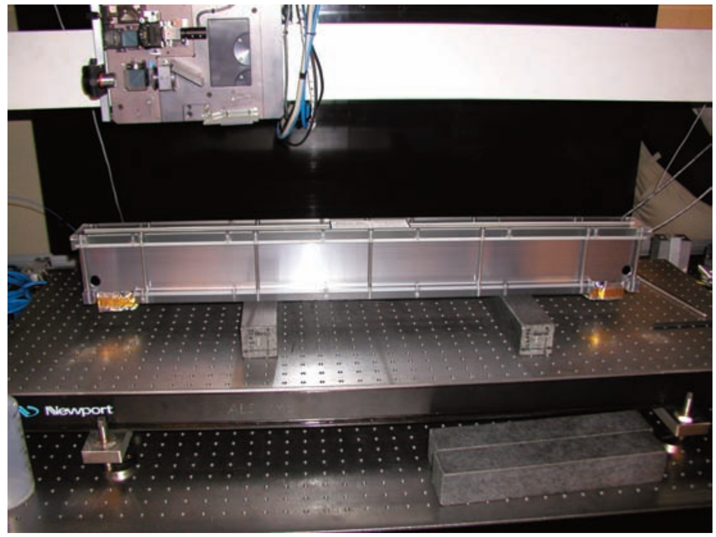
# Structural Biology: $4.8M Upgrade, Complementary Techniques, and the Benefits of Remote Data Collection

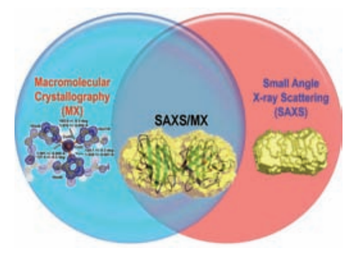
by Paul Adams

The $4.8M upgrade of Beamlines 8.2.1 and 8.2.2, funded by the Howard Hughes Medical Institute, is now entering its final stages with the last of the three new x-ray mirrors successfully completing metrological acceptance tests. This mirror, together with its twin, is now being prepared for installation into the beamline during the ALS October 2010 shutdown. The new mirrors will replace the existing M1 mirrors in both 8.2.1 and 8.2.2 and will enable a significantly tighter focus to be achieved at the sample. These upgrades to the optics take advantage of the reduced vertical beam emmitance resulting from ALS top-off mode. The brightness of the beamline will increase by a factor of five, and together with the excellent stability of the goniometer in the MD2 endstation, the upgrade will allow routine data collection on crystals as small as 10 microns. The final component in the upgrade program, a new liquid-nitrogen-cooled monochromator for 8.2.1, is also nearing completion and is currently undergoing final assembly at the vendor's facility in Oxford, UK. Installation is planned for December 2010.

The atomic to 100-nanometer length scale, bridging the distance between detailed chemistry to cellular organelles, poses a tremendous challenge to our understanding of cellular biology. Yet a mechanistic understanding of disease and microbe metabolism requires a comprehensive perspective at precisely these length scales where an astounding array of dynamic macromolecular machines control cellular fate and function. The ALS and its joint macromolecular crystallography (MX) and small-angle x-ray scattering (SAXS) program (at the SIBYLS Beamline, 12.3.1) have established a leadership role in the hybrid application of both techniques. MX provides unparalleled precision while SAXS provides accurate shape and assembly information on functioning macromolecular machines. Technological developments in MX have revolved around improving the ability to measure ever-smaller crystals with larger imperfections—characteristics of crystals grown from challenging systems that have a high impact. Technological developments in SAXS have revolved around increasing throughput so that macromolecules can be visualized in a host of conditions with a variety of co-factors and in different contexts. The combination has been quite powerful and the structural biology community is now starting to exploit this opportunity.



Beamline 8.2.1 M1 mirror in ALS metrology testing to determine mirror properties such as slope error.




Hybrid application of small-angle x-ray scattering (SAXS) and macromolecular crystallography (MX) experiments at SIBYLS. Left: 0.96-Å resolution active site of Cu/Zn super oxide dismutase (SOD), Right: SAXS envelope of SOD assembly in solution. Center: Atomic-resolution dimer docked into envelope.

The availability of high-reliability crystal sample mounters has transformed protein crystallographic data collection into an experiment in which the locality of the user is determined solely by the length of the network cable. Using remote desktop technology, users from across the world have access to many of the macromolecular crystallography beamlines at the ALS from the comfort of their home institutions. At the Berkeley Center for Structural Biology (BCSB), the level of remote user activity has increased dramatically over the last two years (now more than 50%). Typically, users ship their specimens in special sample holders (pucks) to arrive at the beamline a day before an experiment

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## National Center for X-Ray Tomography

continued from page 8

from being able to change phenotype, thus preventing it from becoming pathogenic. The Stanford team worked with the NCXT to image *Candida albicans* cells with a variety of phenotypes and after treatment with peptoid molecules [Uchida et al., *PNAS* **106**, 19375 (2009)]. These images allowed our first look inside cells before and after treatment with drug molecules.

The NCXT has just been awarded five more years of funding, from both NIH and DOE, to continue advancing soft x-ray tomography as a biological/biomedical imaging technique. The future of this ALS user resource looks very bright indeed. ■

# CXRO: Progress in Imaging, Metrology, and EUV Lithography

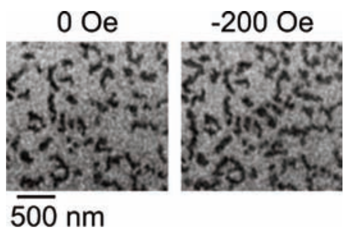
by Patrick Naulleau

Although the Center for X-Ray Optics (CXRO) is part of the Materials Sciences Division (MSD), the Center has a tight and multifaceted relationship with the ALS. The past year has brought many changes and much progress at CXRO. I am honored to now serve as the Acting Director of CXRO and Ken Goldberg, another long-term CXRO member, is now Deputy Director. We very much look forward to continuing and further expanding the close collaborations between CXRO and the ALS.

In the past year, CXRO has again made significant progress both scientifically and technologically in its x-ray imaging,

**Patrick Naulleau**

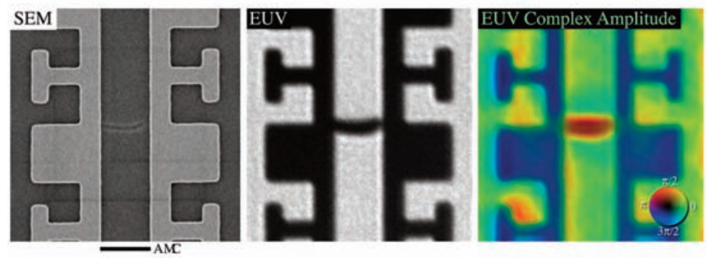
metrology, and industry-funded extreme ultraviolet (EUV) lithography research programs. The research performed at the Center's nanofabrication and coating facilities enables it to provide high-resolution diffractive optics, coatings, and other nanostructures, for its own activities and for the support of numerous ALS activities. In addition to the nanostructures described below, the CXRO multilayer coatings and metrology efforts played a crucial role in the ALS's development of a new high-efficiency blazed grating for monochromators operating at EUV wavelengths.




High-resolution magnetic soft x-ray microscopy of Barkhausen avalanche processes in a 50-nm thin $(Co_{84}Cr_{16})_{87}Pt_{13}$ nanogranular film.

The CXRO nanofabrication facility has developed the world's highest-resolution soft x-ray zone plates. In particular, CXRO zone plates have been used to demonstrate 10-nm resolution in two different instruments at the ALS during this past year. The first example was at CXRO's XM-1 microscope at Beamline 6.1.2, where a 12-nm zone plate fabricated using double patterning methods was combined with a new high-resolution condenser zone plate to achieve 10-nm half-pitch imaging. CXRO zone plates also enable various STXM microscopes operated by the ALS. Recently the CXRO nanofabrication team has pushed STXM zone plates down to 17 nm, yielding 10-nm resolution at ALS Beamline 11.0.2.

The full-field soft x-ray microscope, XM-1, at Beamline 6.1.2 is a unique analytical tool for nanoscience research, combining excellent spatial and temporal resolution (70 ps) with a rich set of contrast mechanisms: 




EUV amplitude and phase images (center and right) of a native defect on an EUV mask compared to a scanning electron micrograph (left).

elemental, chemical, topological, and magnetic. Nanomagnetism research using XM-1 is focused on a fundamental understanding of magnetic properties at fundamental length and time scales. Over the past year, high-resolution studies at XM-1 of Barkhausen avalanches in a nanogranular magnetic CoCrPt film indicated a clear stochastic character. This finding is very important since it implies fundamental limits in the ability to deterministically switch these nanoscale magnetic bits. Continued research in this area is crucial and potentially a rich area for a next-generation light source (NGLS). In addition to being the cornerstone of CXRO's nanomagnetism research, XM-1 also supports a vibrant ALS user program.

CXRO's extreme ultraviolet lithography (EUVL) research tools provide the semiconductor industry with imaging capabilities generations ahead of their current processes. The SEMATECH Berkeley Micro Exposure Tool (MET) on ALS Beamline 12.0.1.3 provides the world's highest-resolution EUV printing capability for evaluating photoresist materials and for mask research. The MET drives resist innovations in the areas of resolution, sensitivity, and line-edge roughness, with hundreds of new resist formulations being tested every year. At the neighboring Beamline 11.3.2, the SEMATECH Berkeley Actinic Inspection Tool (AIT) is a unique EUV Fresnel zone-plate microscope dedicated to photomask research. The AIT images the reflective surface of EUVL masks, characterizing defects and the wavelength-specific optical properties of circuit patterns the masks are designed to reproduce. As the highest-performing tool of its kind, the AIT serves researchers from the leading semiconductor companies, providing fundamental learning not available anywhere else. As shown the figure, the capabilities of this tool have recently been expanded to include quantitative phase imaging.

Although we are independent, CXRO and the ALS enjoy a synergistic relationship. I look forward expanding this relationship and the bright future we will create together. ■

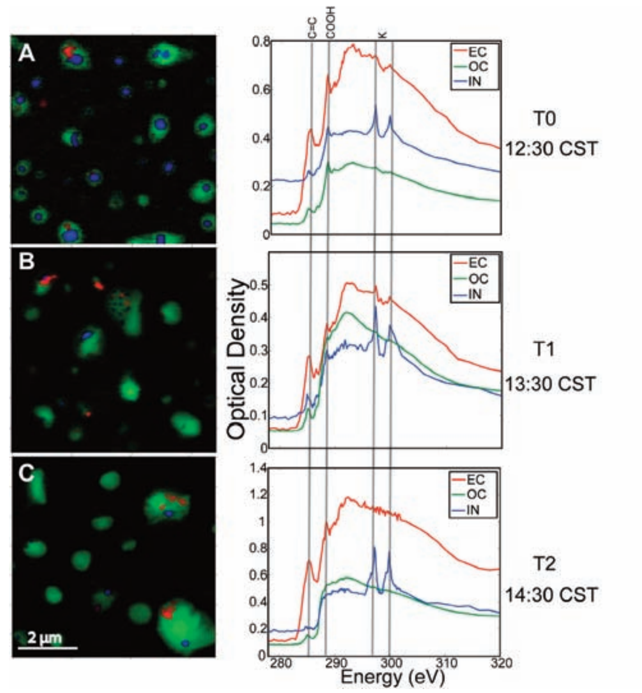
# Studies of Atmospheric Aerosols and Catalysis at Beamline 11.0.2

by Hendrik Bluhm, Mary K. Gilles, Tolek Tyliszczak, and David K. Shuh

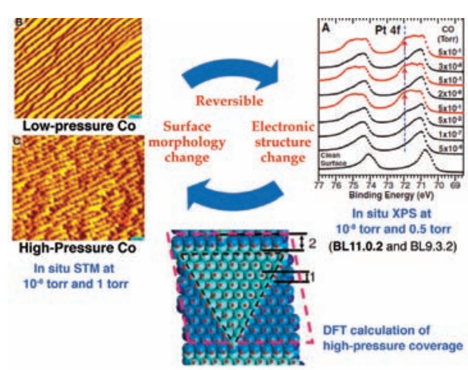
Beamline 11.0.2, the ALS Molecular Environmental Science (ALS-MES) beamline, continues to be productive scientifically while technical advancements for existing and new endstations continue. Work at the STXM endstation is split into experiments involving soils, catalysis, stardust, actinides, energy, atmospheric aerosols, and studies of the magnetic properties of materials. One particular outstanding characteristic of the ALS-MES STXM has been its state-of-the-art spatial imaging, and continual improvements have recently resulted in a record 10-nm resolution. Ambient-pressure photoemission spectroscopy (APPES) endstation experiments focus on environmental, catalysis, and energy sciences. Development of a second ambient-pressure system, allowing users to connect an external endstation to an ambient-pressure photoelectron spectrometer, will expand the types of experiments performed.

In recent years, investigations of atmospheric aerosols have been of increasing interest, and studies exploring metal oxidation states, oxygenated coatings on aged biomass burn aerosols, and sulfur speciation are summarized in a recent book chapter ["Scanning Transmission X-ray Microscopy: Applications in Atmospheric Aerosol Research," by R.C. Moffet, A.V. Tivanski, and M.K. Gilles in *Fundamentals and Applications of Aerosol Spectroscopy,* Taylor and Francis Books, Inc. (to be published in 2010)].

Determination of the changing composition of carbonaceous particles, and in particular the ability to isolate soot within individual particles, can be uniquely done using STXM. In a recent study, particles were collected at three sites in and around Mexico City. Samples were chosen for comprehensive analysis from a day when the same air mass traveled through each site. The particle components—soot (elemental carbon), inorganic, and organic—were identified by their NEXAFS spectra and used to quantify trends in particle mixing from the three sampling sites progressively further from the city. The data illustrate the complex mixtures of components within particles at the city center. Farther from the city center, the number fraction of homogenous organic particles lacking both soot and inorganic inclusions increased. Although these particles lacked organic inclusions, examination of the sulfur-edge spectra showed that inorganic sulfate was homogenously mixed with the organic material. Understanding how these different components are mixed within individual particles as well as the ensemble of particles provides the benchmarks necessary to improve models of the atmospheric aging of soot. Soot is the primary atmospheric species that absorbs solar radiation, and how it is mixed with other components within a particle can change its optical absorption by as much as a factor of three. Hence, the ability to monitor changes is critical for providing feedback necessary to improve climate-change models.




(A)–(C) display maps of the carbonaceous spectral components shown on the right. Atmospheric aerosols were collected at (A) a source at the center of Mexico City (T0), (B) ~1 h north (T1), and (C) ~2 h north (T2). EC = elemental carbon, IN = inorganic, OC = organic. In A, the blue IN (primarily K) cores are surrounded by green OC regions. Mixed in are red soot inclusions EC. With increasing distance from the source region, the organic component dominates the particle composition, indicating photochemical atmospheric processing [R. Moffet et al., *Atmos. Chem. Phys.* **10,** 96 (2010)].




Reversible differences in the surface morphology and corresponding electronic structure of the CO-Pt interface at CO pressures of $10^{-8}$ Torr and 1 Torr. The experimental results are supported by DFT calculations that confirm the structure observed at high pressure [F. Tao et al., *Science* **327**, 850 (2010)].

Combined ambient-pressure XPS (Beamlines 11.0.2 and 9.3.2) and scanning tunneling

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# THE ALS COMMUNITY

by Roger Falcone

## Renewing the ALS

I am pleased to report on a successful and auspicious year for users at the Advanced Light Source. The number of proposals, publications, and users are all increasing, and the quality of research remains extremely high. We are grateful for the Department of Energy's strong support of both our mission and our goals for the future. I continue to be grateful for our ALS staff as they undertake the challenging yet rewarding work of new projects while also enabling current users. Finally, I'm particularly appreciative of the continued dedication of ALS users, in helping us make sure that the ALS remains the best facility for their research.

We have now benefited from the second year of significant DOE investments in renewing the ALS, renewal by way of new technology such as detectors at our beamlines, in increased funding for operations, and in support for modernizing our storage ring.

Last year, we received funding for construction of MAESTRO, our new angle-resolved, high-spatial-resolution photoemission beamline, as well as funding under ARRA (American Recovery and Reinvestment Act), which accelerated construction of the User Support Building and built new instruments on the ALS floor. Work on all these projects is going well.

This year, we were awarded resources to begin work on COSMIC, the first ALS beamline optimized for coherence applications. Additionally, we received infrastructure support for expanding our efforts in optical metrology, which is necessary to keep our x-ray optics at the technological frontier, as well as funding to replace the critically important controls system and power supplies.

These renewal funds are necessary to keep the ALS world-leading in soft x-ray science. They also support the ever-increasing number of user proposals and demand for beam time, as well as additional scientific, technical, and administrative staff, who are seeing increasing demands on their time and heavier workloads.

Planning for our many new projects is part of the job of our two excellent deputy directors: Bob Schoenlein (for science), who joined us last year, and Michael Banda (for operations) who joined us this year. Banda, who took over from long-time ALS deputy Ben Feinberg, was previously the deputy in computing at Berkeley Lab and is a biologist. We are very fortunate that Ben and former ALS director Janos Kirz remain close to ALS as advisors, while spending much of their retirements engaged in their exciting science programs at the Lab.

ALS staff and users are fully participating in Berkeley Lab's two major new initiatives: Carbon Cycle 2.0 and a next-generation x-ray laser facility. These activities are at the forefront of Director Paul Alivisatos's strategic vision for the Lab. A relevant new publication—Photon Science for Renewable Energy—was developed by ALS scientists and users, working together with the ALS Communications Group. I urge you to pick up a copy of this green booklet from the ALS lobby, read how the ALS is contributing to energy research within CC2.0 and addressing climate change, and see how you might get involved. We also invite ideas for the science and technology that would be enabled by a new, powerful, fully coherent, soft x-ray laser source.

Personally, I continue to benefit enormously from feedback from users, often channeled through the Users' Executive Committee, as we operate and undertake the renewal of our light source. Renewal concepts are outlined in the ALS Strategic Plan, which was developed over several years and is available on the ALS Web site. I hope you share my enthusiasm as we realize these strategic planning goals. ■

## R&D 100 Winner: APPELS

An international collaboration that included ALS scientists Frank Ogletree, Hendrik Bluhm, Zahid Hussain, and Miquel Salmeron developed a novel lens system that makes possible the use of x-ray photoelectron spectroscopy (XPS) technology under pressures and humidities similar to those encountered in the natural environment. Called the Ambient Pressure PhotoElectron Lens System (APPELS), this new technique has already led to groundbreaking discoveries in climate change, atmospheric science, nanotechnology, and industrial processes, such as heterogeneous catalysis.

XPS is typically performed in a vacuum or at pressures below 4.6 Torr, which is the scientifically and technically important vapor pressure of water at

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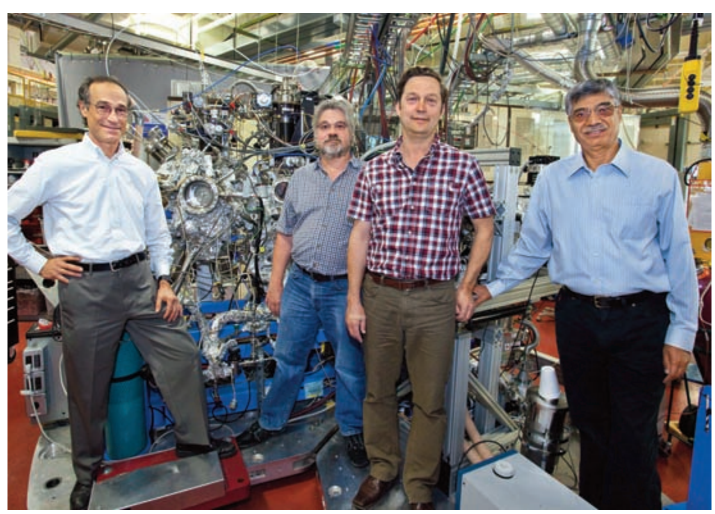


Berkely Lab members of the APPELS team (L-R): Miquel Salmeron, D. Frank Ogletree, Hendrik Bluhm, and Zahid Hussain.

THE ALS COMMUNITY

## Users' Executive Committee Update

by David L. Osborne, 2010 UEC Chair

It is my pleasure to serve the users of the ALS as chair of the Users' Executive Committee in 2010. In the past year, over 2000 researchers have used more than 30 beamlines at the ALS to advance fundamental scientific knowledge in areas as diverse as combustion chemistry, protein crystallography, topological insulators, biological imaging, photolithography, and catalysis, to name just a few areas. This incredible variety of research, accomplished by external users and ALS scientists, could not happen efficiently and safely without the consistent efforts of management and support staff at the ALS. They deserve our thanks for continuing to advance this incredibly complex operation.

The 11 members of the Users' Executive Committee (UEC) represent the interests of users to both the Department of Energy and ALS management. The ALS management turns to us first, whenever decisions that impact users must be made, and we work closely together to make sure that the needs and perspectives of users are always at the forefront. Whenever user issues arise, please feel free to contact me or the other UEC representatives.

We all recognize that one group's safety issues can adversely affect the entire user community. Building on the success of the 2009 Health and Safety Security Audit, Jim Floyd and his safety team have continued to provide thoughtful advice and solutions to the myriad safety challenges that a densely populated, open environment like the ALS poses. Their "can do" attitude combined with a willingness to help in a timely manner keeps science flowing at a rapid pace while maintaining a safe environment for all of us.

I am happy to report that the Berkeley Lab Guest House has been in operation for almost one year, providing a convenient housing option (with an amazing view) to anyone working at the ALS or Berkeley Lab. The addition of off-hours, free taxi service to and from downtown Berkeley and food delivery from many restaurants directly to the Guest House makes this facility a great way to maximize the effectiveness of visiting scientists.

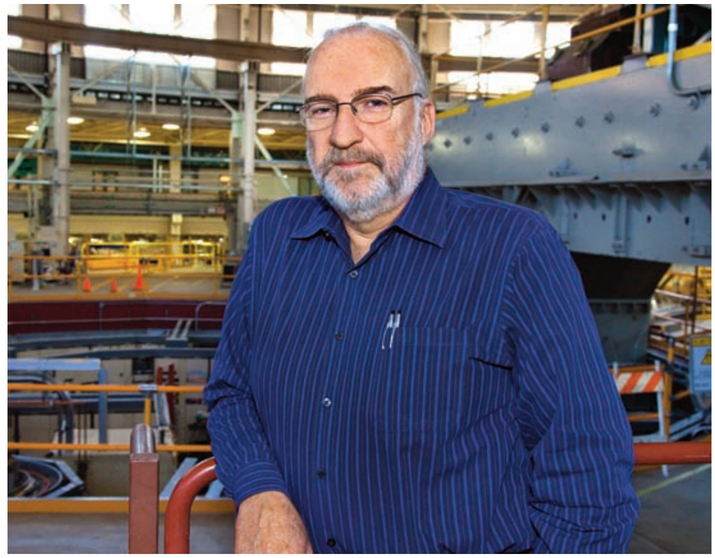
In addition, the new User Support Building (USB) opened its doors in late summer of 2010. Providing major improvements in experiment staging and assembly, new staff offices, user drop-in cubicles, lockers for user storage, increased meeting space, and increased parking (!), the USB will be a significant step forward in the way the ALS serves its scientific community. The users, through the UEC, have been strong advocates for both of these new buildings, and we will be proud to see them both in operation.

Every year, the planning and execution of the ALS Users' Meeting is the main activity of the UEC. This year program co-chairs, Hendrik Bluhm and Brandy Toner, together with Sue Bailey, Deborah Smith, and their team at the ALS User Office, have organized an exciting meeting. We hope you can join us October 13–15, 2010, to see the accomplishments of the past year and contribute to new research directions though the many topical workshops.

Finally, I would like to thank Ken Goldberg, past UEC chair, and my colleagues on the UEC for their commitment to the user community. Being on the UEC is a great way to serve the user community and raise the profile of your group's work. I would encourage any user to become involved with the UEC—consider running for office this year to help shape the future of science at the ALS!

As we help solve the scientific needs of our nation and world, I wish you the best for a productive year of research. ■

## Michael Banda, New Division Deputy for Operations



Michael Banda has been named as the new ALS Division Deputy for Operations (DDO). "Banda," as he prefers to be called, has been with Berkeley Lab since 1999. He began as the Division Deputy for Life Sciences, then became the founding Division Deputy for Genomics at the time when the Joint Genome Institute (JGI) was formed. In 2001, Banda moved on to become Division Deputy for Computing Sciences, where he held responsibilities with the Computational Research Division and the National Energy Research Scientific Computing Center (NERSC).

His previous work with x-ray science includes an appointment as Director of the Laboratory of Radiological Biology at the University of California, San Francisco, a unit that studied the effects of radiation in applications of biochemistry and cell biology.

As the DDO, Banda will manage the overall operation of the ALS, including accelerator and beamline operations, user activities, safety, and environmental protection activities. He will be working directly with ALS Operations, Engineering, and Business Management Groups. Banda sits in Ben Feinberg's old office (80-228), and can be reached at MJBanda@lbl.gov or x2837. ■

## THE ALS COMMUNITY

# Honors and Awards

**Thomas Steitz,** Yale University and Howard Hughes Medical Institute, a regular user of structural biology Beamlines 8.2.1 and 8.2.2 at the ALS, received the 2009 Nobel Prize for Chemistry (with Venki Ramakrishnan and Ana Yonath) for studies of the structure and function of the ribosome. At the ALS, Steitz has performed crystallographic experiments at Beamline 8.2.2 to understand the mechanism of antibiotic resistance by eubacterial ribosomes, resulting in the publication of "Structures of MLSBK antibiotics bound to mutated large ribosomal subunits provide a structural explanation for resistance," D. Tu, G. Blaha, P.B. Moore, and T.A. Steitz, *Cell* **121**, 257 (2005). In addition, each Nobel announcement includes supporting documentation outlining the case that the Nobel committee considered in coming to their conclusion. Two of our users, Jamie Cate (University of California, Berkeley) and Harry Noller (University of California, Santa Cruz) were widely cited for their pioneering structural work on the ribosome, including the first solution of the intact ribosome structure to atomic resolution.

**Zhi-Xun Shen,** Director of the Stanford Institute for Materials and Energy Science (SIMES), has been awarded the Ernest Orlando Lawrence Award by the U.S. Department of Energy for his pioneering work in materials science. Shen has been a very active user of the ALS and has carried out much of his research at ALS Beamline 10.0.1. Shen's award, announced on December 16, 2009, is "for his ground breaking discoveries and pioneering use of high resolution angle-resolved photoemission to advance understanding of strongly correlated electron systems including high-transition temperature superconductors and other complex oxides." It is one of the highest scientific honors bestowed by the U.S. government.

The editors of the scientific journal, *Nuclear Instruments and Methods in Physics Research, Section A*, have awarded to **Eli Rotenberg** (ALS Scientific Support Group Deputy Leader) the first Kai Siegbahn Prize, named in honor of the journal's founder. The award citation recognizes Eli for "the creation and development of the 'Electronic Structure Factory' end-station at the Advanced Light Source, which could legitimately be called the most useful ARPES end-station in the World. This endstation has been used to tease out many first results in a wide variety of complex and exotic materials. Eli Rotenberg's artful application of ARPES has greatly contributed to the understanding of some of the quantum electronic properties of nano-phase and reduced dimensionality materials. His scientific achievements are reported in tens of publications on the most prestigious journals of physics and scientific magazines."

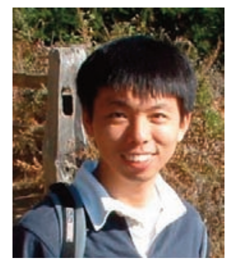
Steitz

Shen

Rotenberg

Lanzara

Ramesh



Wang

At the March 2010 American Physical Society Meeting, the following scientists, who have performed extensive research at the ALS, were acknowledged for their groundbreaking work: **Alessandra Lanzara**, University of California, Berkeley, and Berkeley Lab: 2010 Maria Goeppert Mayer Award for "High-resolution angle-resolved photoemission spectroscopy and imaging studies of the cuprate superconductors and graphene that elucidate their electronic properties." **Ramamoorthy Ramesh**, University of California, Berkeley: 2010 James C. McGroddy Prize in New Materials for "Groundbreaking contributions in theory and experiment that have advanced the understanding and utility of multiferroic oxides." **Feng Wang**, University of California, Berkeley: IUPAP Young Scientist Award for "Bilayer graphene: Tunable bandgap and electron-phonon Fano resonances." **Eli Rotenberg**, Berkeley Lab: VUVX (Vacuum UltraViolet and X-Ray) Conference Award for "his outstanding contributions to angle-resolved photoemission with synchrotron radiation in the study of surfaces and electronic structure."

**Feng Wang** was also named a Department of Energy Office of Science Early Career Research Program Award Winner for "Control of Graphene Electronic Structure for Energy Technology," funded by the Office of Basic Energy Sciences. **René Bilodeau**, Western Michigan University and Berkeley Lab received the Yong-Ki Kim Award for Excellence in Research Post Doctoral Award for the paper "Promoting a core electron to fill a d shell: A threshold law and shape and Feshbach resonances." **Elke Arenholz** was elected as vice chair of the IEEE Oakland-East Bay Section Magnetics Society Chapter. **Zahid Hussain** was appointed as a Consulting Professor of Photon Science at SLAC National Accelerator Laboratory. ■

THE ALS COMMUNITY

## ALS Attracts High-Profile Visitors

The ALS remains a must-see stop for visitors to Berkeley Lab, hosting tour groups representing scientific, governmental, educational, and community interests.

Members of the Executive Committee of the France-Berkeley Fund (FBF) met on the UC Berkeley campus the morning of May 24 to review applications for grants, then came up to Berkeley Lab for tours of the Molecular Foundry and the ALS guided by Ben Feinberg and Michael Banda. Established in 1993 as a partnership between the government of France and the University of California, Berkeley, the FBF promotes scholarly exchange in all disciplines between UC Berkeley and all research centers and public institutions of higher education in France.

On May 19, Sally Ericsson, the Program Associate Director for Natural Resources Programs in the Office of Management and Budget (OMB) at the White House, visited Berkeley Lab and the ALS. Accompanied by Kevin Carroll, Chief of the Energy Branch at OMB, Ms. Ericsson stopped by Beamine 12.0.1.3 to hear from Ken Goldberg about recent advances in EUV lithography.

California Congressman John Garamendi addressed the Berkeley Lab community before touring the ALS with Physical Biosciences Division Director Paul Adams, who gave an overview of the macromolecular crystallography beamlines as well as current energy research at the ALS. The group also stopped by Beamline 6.0 to talk with student Tanja Cuk about artificial photosynthesis. Garamendi serves on the House of Representatives Committee on Science and Technology.

Students from Case Western Reserve University in Cleveland, Ohio, visited the ALS on April 2. Escorted by ALS tour guides Jinghua Guo and Liz Moxon, the students—members of the Physics and Astronomy Club—visited several beamlines and spoke with ALS researchers before taking pictures atop the booster ring.

In early April, Representative Rodney Frelinghuysen, the Ranking Republican Member of the House Energy and Water Development Appropriations Subcommittee, toured Berkeley Lab with stops at the Molecular Foundry, National Center for Electron Microscopy, and the ALS. The subcommittee on which he sits is responsible for writing the annual appropriations bill that funds the Department of Energy.

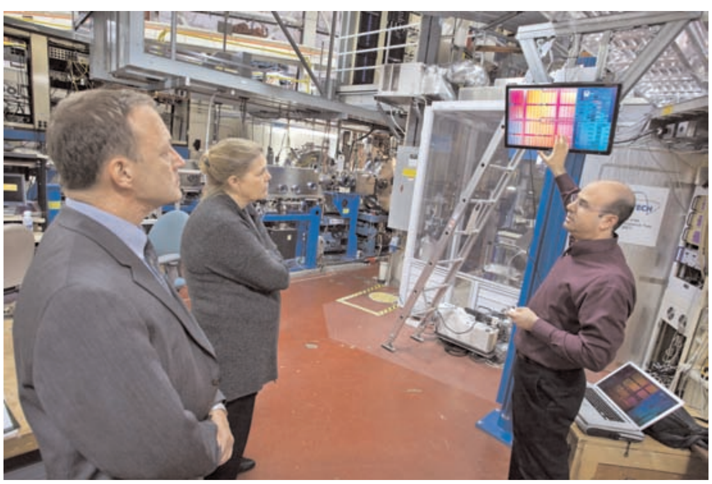
ALS Project Manager Steve Rossi hosted a group of visitors from Kazakhstan on March 5. The visitors, including a representative from the Kazakhstan Embassy in Washington and the President and the Business Development Manager of the New University of Astana, were touring Berkeley Lab to explore the possibilities of developing collaborations and future cooperative agreements.

University of California Regent Ronald W. Stovitz visited the ALS on March 1 as part of a tour of Berkeley Lab. Accompanied by 11 guests, Regent Stovitz was welcomed to the facility by SSG Group Leader Zahid Hussain before touring the experiment floor and visiting beamlines and beamline scientists, Corie Ralston, Eli Rotenberg, and Hendrik Bluhm.

Members of lightsources.org took time out from their meeting at SLAC to tour the ALS on February 24. After a brief welcome by ALS Division Director Roger Falcone, the group visited several beamlines with User Services Lead Sue Bailey. The group, representing synchrotron and FEL sources around the world, promotes the science and technology of light sources through outreach activities and the collaborative Web site *lightsources.org*.

Lawrence Gumbiner, Deputy Assistant Secretary of State for Science, Space, and Health, toured the ALS on January 21 with Deputy Division Director for Operations, Ben Feinberg. Mr. Gumbiner is interested in science policy and in exploring ways to strengthen ties between the State Department and the science and innovation com-

*continued on page 16*



Sally Ericsson (center) and Kevin Carroll (left) from the White House OMB at Beamline 12 with Ken Goldberg (right).

Left to right: Tanja Cuk, Marcus Hertlein, Paul Adams, and Rep. Garamendi.

FACILITY UPDATES

# Accelerator Availability and Reliability

by David Robin

The ALS operating schedule is divided into user beam shifts, accelerator physics/machine setup shifts, maintenance and installation, and vacation shutdown shifts. In a "typical year," there is usually one long shutdown for major servicing, large installations, and upgrades. This long shutdown and associated startup usually occurs in the spring and lasts about six weeks. Also, in a typical year the ALS schedules and delivers more than 5000 beam hours to users. Below is a summary of events during the previous three fiscal years and the availability and reliability of the facility.

Availability is one of the most important performance parameters of the facility. Availability is defined as the ratio of delivered versus scheduled user time. Maintaining a high availability as the facility becomes more mature and complex (e.g., the addition of new insertion devices, feedback and feed forward, injector upgrades and top-off injection) is a challenging task.

The number of hours scheduled and delivered is shown in table. In this review period, there was a deviation from the typical yearly shutdown pattern as described above. In FY07 the ALS had two long-term shutdowns. The first was in the fall of 2006 for the installation and replacement of components necessary to go to full-energy injection in preparation for top-off operation and the other in the spring of 2007. Therefore, the number of scheduled and delivered user hours was lower in FY07 as compared with FY08 and FY09, when there was only one major shutdown.

There was a drop in availability in FY07, a partial recovery in FY08, and a full recovery in FY09. The drop in availability was because of two cascading effects that arose from the injector upgrade. In the fall of 2006, the ALS underwent a major shutdown to install and commission components necessary for full-energy injection. At the end of the shutdown, there was a major failure in one of the components (the booster bend power supply), which resulted in a loss of nine user days. The second effect was that this failure resulted in longer fill times for the remainder of FY07 and FY08. The recovery of the availability to 96.5% in FY09 was somewhat unexpected and exceeded our expectations. The reason being that in February of FY09, the ALS began operating in top-off injection mode and has been doing so nearly full time ever since. There was remarkably no significant teething period in the top-off transition. In fact, the availability in top-off operation was higher (>97%) in FY09 than before top-off operation.

Reliability is another important performance parameter of the facility, which is distinct from availability. Reliability is defined as the ratio of the number of actual fills that were completed without interruption versus the number of scheduled fills. Providing good availability is necessary but not sufficient to ensure good reliability. For example, a user run with many unscheduled dropouts but fast recovery times would result in good availability but poor reliability. A good measure of reliability is the mean time between failures (MTBF). The MTBF was 51 hours in FY07, 46 hours in FY08, and 41 hours in FY09. This downward trend is directly linked to increased failure of aging components. We are addressing this issue by systematically replacing critical components. ■

**HOURS SCHEDULED AND DELIVERED**

| | Scheduled hours | Delivered hours* | Availability | Mean time between failures (hours) |
|---|---|---|---|---|
| FY07 | 4200 | 3864 | 92.0% | 51 |
| FY08 | 5000 | 4664 | 93.3% | 43 |
| FY09 | 5471 | 5278 | 96.5% | 41 |

*Does not include unscheduled hours delivered to users.

THE ALS COMMUNITY

## High-Profile Visitors

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munity in Northern California.

Carl Bauer, Special Assistant to the Assistant Secretary of Fossil Energy, DOE (formerly Director of NETL) and Jim Wood, Deputy Assistant Secretary for Clean Coal, were given a tour by SSG Leader Zahid Hussain.

Roland Sauerbrey, the Scientific Director at Forschungszentrum Dresden-Rossendorf toured the ALS experiment floor with Ben Feinberg on January 6.

Representative Bill Foster, one of only three physicists in the U.S. Congress, spoke on "What It's Like to be a Scientist in the U.S. Congress" at Berkeley Lab on Monday, November 9. Foster, a researcher at Fermilab for 22 years, helped discover the top quark, the heaviest known form of matter. As part of his visit, Rep. Foster toured the ALS with Director Roger Falcone. The congressman was particularly interested in Alastair MacDowell's effort on measuring $CO_2$ transport through rock on Beamline 8.3.2, in connection with the Lab's work on energy and climate change related to carbon sequestration. Foster was also interested in Berkeley Lab's proposed new x-ray FEL source.

Members of the Australian Parliament toured the ALS with Roger on September 28. The delegation was led by Senator John Hogg, President of the Australian Senate (equivalent to the U.S. Speaker of the House). In addition to visiting the ALS, the delegation toured the National Center for Electron Microscopy (Uli Dahmen) and heard presentations on advanced biofuels development (Jay Keasling) and energy-efficient buildings (Arun Majumdar/Steve Selkowitz). ■

# FACILITY UPDATES User Demographics and Publications

by Sue Bailey

As a national user facility, the ALS is required to report user demographics and publication information annually to the U.S. Department of Energy. Figure 1 shows the breakdown of different types of institutions that make up our user base. Figure 2 shows the overall user numbers in various scientific fields over time (FY00–FY09). The overall number of users at the ALS has stabilized at around 2000 following the effects of two shutdowns that occurred in FY07. The scientific productivity of the ALS as measured in refereed and high-profile publications since 1994 is shown in Figure 3. To improve consistency in this measure, we now count "refereed journal articles" as opposed to the previous "refereed publications," a category that was not well defined. ■

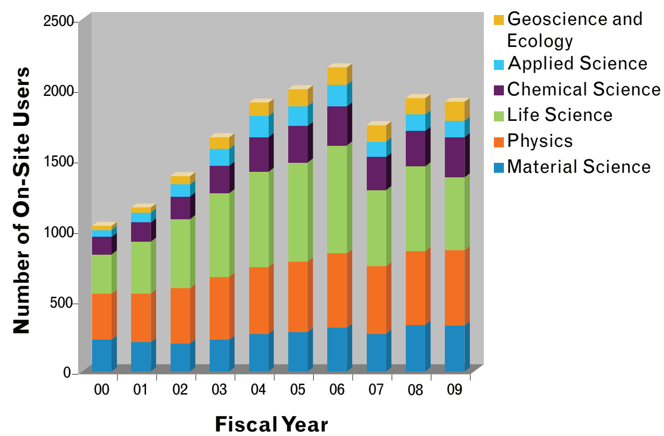



Figure 2. Bar graph showing the relative numbers of on-site users in various areas of science.

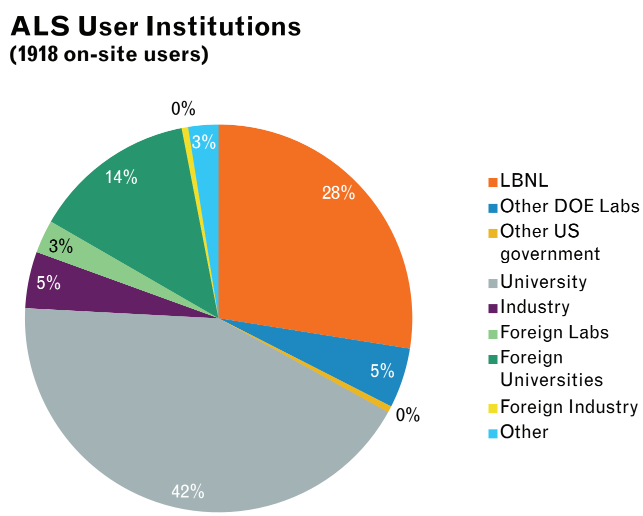



Figure 1. Pie chart showing percentages of different types of user institutions.

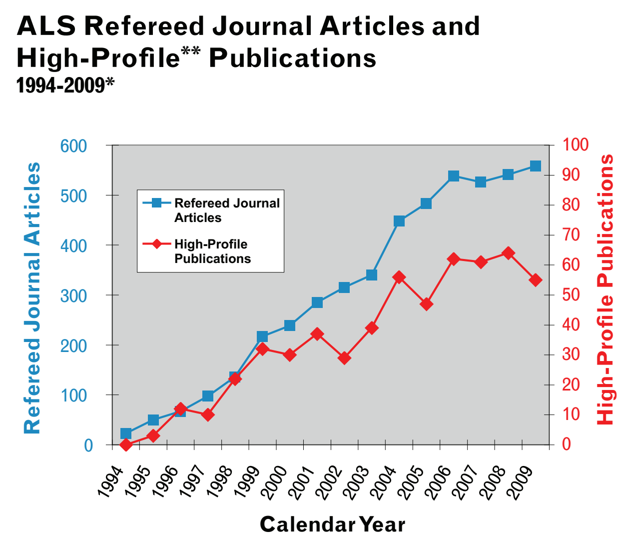



Figure 3. Graph of growth in refereed journal articles (blue) and high-profile publications (red). *Note that publications for 2009 were still being collected at the time this section was being written. **High-profile publications include *Nature*, *Science*, *PRL*, and *Cell*.

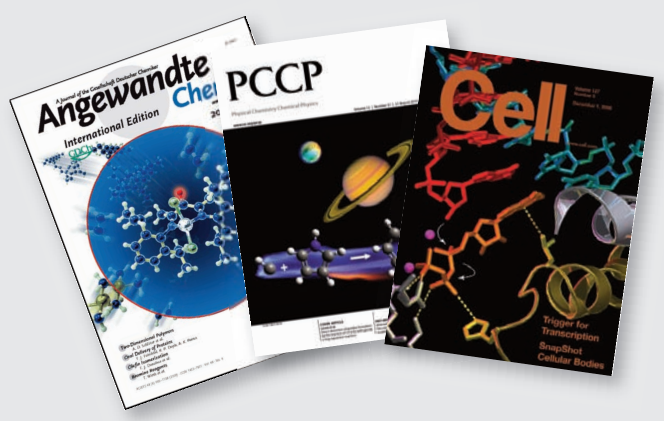
## Be Counted—Submit Your Publications ASAP!

If you have recently done any of the following based on work done at the ALS, let us know as soon as possible:

- ✓ Published ALS-related work in a scientific journal or book chapter
- ✓ Received a patent
- ✓ Completed a Ph.D. thesis
- ✓ Received an award
- ✓ Given an invited talk

Publications are a primary metric used by DOE in the funding process. Remember, if it's on your CV and all or part of the work was done at the ALS, it should be in our database!

Check the ALS Web site, *www.als.lbl.gov*, for more information.



## Science Roundup

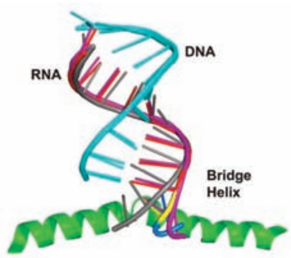
continued from page 4

shells and xenon (Xe) cores. The clusters were site-selectively ionized (i.e, ionization took place either in the xenon core or in the argon shell). Using a high-resolution photoelectron–ion coincidence technique at ALS Beamlines 10.0.1 and 11.0.2, the researchers concluded that charge-transfer processes and fragmentation dynamics are strongly influenced by the environment of the initially ionized atoms.

### Proofreading RNA: Structure of RNA Polymerase II's Backtracked State

Wang et al., *Science* **324**, 5931 (2009)

For genes to be expressed, a complementary strand of RNA must be produced from a DNA template. During this process of transcription, a special class of enzyme called RNA polymerase moves along the DNA template, reading the DNA and producing an RNA complement. This process operates with amazingly high fidelity—the error rate is as low as one mistake for every 100,000 DNA base pairs transcribed—thanks in part to error correction by an RNA polymerase known as pol II, which "backtracks," or reverses, along the transcript to remove misincorporated or damaged nucleotides. A group from the Stanford University School of Medicine has solved the structure of pol II in the backtracked state, providing structural insights about a key mechanism for ensuring accurate transcription.

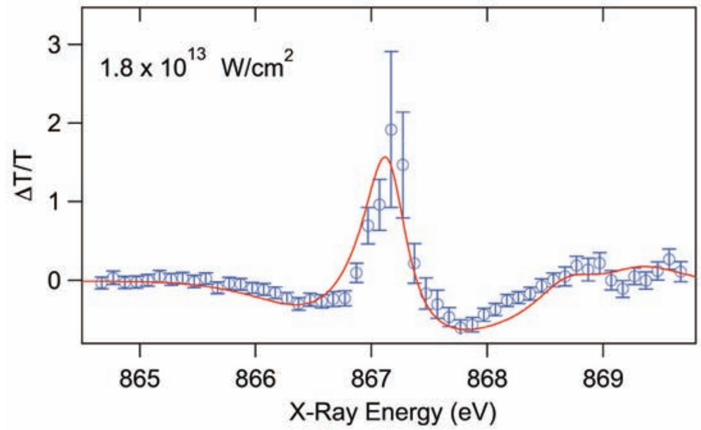



Backtracked RNA is kinked toward the bridge helix and differs from the canonical form of RNA. Backbones of one-base–mismatch backtracked RNA (red, yellow, and blue) and canonical form RNA (gray) are superimposed. The superimposed two-base–mismatch structure is shown in magenta.

### Using Light to Control How X Rays Interact with Matter

Glover et al., *Nat. Phys.* **6**, 69 (2009)

Schemes that use one light pulse to manipulate interactions of another with matter are well developed in the visible-light regime where an optical control pulse influences how an optical probe pulse interacts with a medium. This approach has opened new research directions in fields like quantum computing and nonlinear optics, while also spawning entirely new research areas, such as electromagnetically induced transparency and slow light. However, it has been unclear whether similar optical control schemes could be used to modify how x rays interact with matter. In a dramatic breakthrough demonstration at the ALS, a Berkeley Lab–Argonne National Laboratory group has now used powerful visible-light lasers to render a nominally opaque material transparent to x rays. While x-ray transparency will have immediate applications at x-ray light sources, the important result is that the findings lay a foundation for a broader spectrum of applications. ■




Example of optically induced x-ray transparency data. The laser (~1.55 eV) coherently couples core-excited 3s and 3p states, thereby inducing transparency on the 1s → 3p x-ray absorption resonance. The solid line shows the theoretical simulation of the expected change in transmission. The degree of transparency varies linearly with intensity within error.

## APPELS

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the triple point and the critical threshold pressure for environmental science studies. Through a technique called pressure differential pumping, the APPELS technology allows measurements at pressures of more than 10 Torr. This enables investigators using APPELS to improve climate-change models, ward off the damaging effects of humidity on nanosystems, provide insights into the impact of chemicals on agricultural plants and human health, and aid in controlling the pollution of air, water, and other environmental systems. With APPELS, it is possible to observe chemical interactions at the atomic level for gas/liquid and liquid/solid interfaces at ambient pressures.

APPELS is now part of XPS instruments being used on two beamlines at the ALS and on beamlines at other synchrotrons around the world, including the National Synchrotron Light Source at Brookhaven National Laboratory, BESSY and the Centre for Synchrotron Radiation in Germany, the MAX-Lab synchrotron in Sweden, and the ALBA synchrotron in Spain. In addition, Sweden's Gammadata is offering an instrument that relies on APPELS technology. APPELS was developed with support from the DOE Office of Science, with additional support from Berkeley Lab's Laboratory Directed Research and Development (LDRD) program. ■

## User Support Building

*continued from page 1*

area has roll-up door access to both the adjacent roadway and the ALS experiment floor. The first floor also contains mechanical assembly areas; user chemistry, mammalian cell, and yeast cell labs; and locker storage.

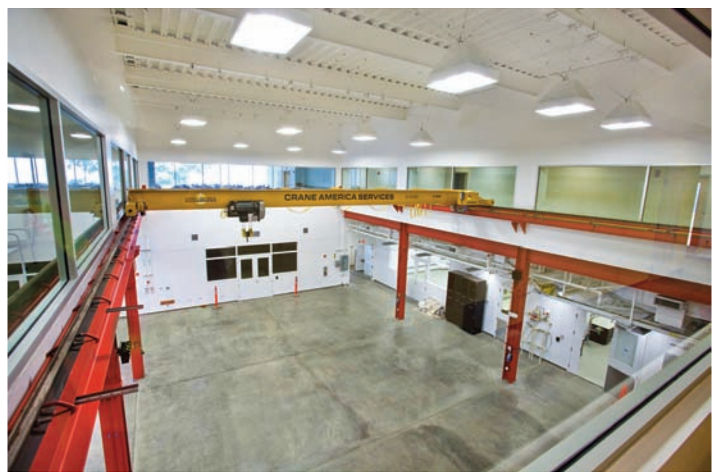
The second floor contains 16 enclosed offices and a state-of-the-art server room with 18 full-height water-cooled racks, as well as an 80-person-capacity conference room, lounge area, and outdoor patio that all boast some of the best views of the San Francisco Bay Area anywhere. The third floor has an additional 15 offices, a smaller boardroom-style conference room, another patio and lounge with those same stellar views, and a high-quality open office area with desk space for 48. The open office area is unique in its quality due to the high ceilings, skylights, ergonomic furniture, and noise masking system. The open office area will have both assigned spaces for our longer-term users and guests as well as drop-in spaces to meet the needs of those at the ALS for less than a month at a time.

Aside from housing support for a state-of-the-art science program, the building itself is state-of-the-art in terms of both structural design and sustainability. The structural design needed to account for both the Lab's proximity to active fault zones and our program's need for the large open space that is the staging area. To address these issues, the design is a moment frame steel structure resting on 57 piers that were drilled down to bedrock. In case of a seismic event, the moment frames allow the building to move and twist up to six inches in any direction as well allowing for significant inter-story drift to prevent major damage and collapse.

Sustainability was considered throughout the design and construction process with the goal of achieving a Leadership in Energy and Environmental Design (LEED) rating of "Silver," and opportunities in the process arose such that the building may yet receive a "Gold" rating when the administering agency, the U.S. Green Building Council, completes its review of the submitted documentation. Energy efficiency plays a major part in LEED certification and is a major challenge in the design and construction of buildings that contain things like fume hoods and server rooms. The design team rose to the challenge and identified opportunities such as utilizing existing capacity in both the ALS boiler and cooling plants, hence eliminating these items from the USB. Minor modifications to these plants also enabled greater efficiency out of the plants, lowering the total energy utilized by the ALS itself.

After many years working on the User Support Building, it is wonderful to look at our exciting new facility and know that is it finally serving the ALS community and will be doing so for many years into the future. Please be sure to come by and check out the facility the next time you're at the ALS. ■

The completed ALS User Support Building front entrance, with ALS dome in the background.




View of high bay from second-floor balcony of the new User Support Building. Chemistry labs are located on the first floor, along the far wall.

The second-floor lounge area with expansive view of San Francisco Bay is separated from the main conference room by a wall of floor-to-ceiling windows.

## Structural Biology

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starts. When the data collection runs starts, beamline staff members load the pucks into a robot and enable remote control of the beamline for the designated user group. The availability of 22-hour BCSB onsite support throughout the working week allows the remote users to have pucks changed out in a timely fashion regardless of the time zone in which they are located. In a research environment where budgetary constraints on travel are common, remote access can reduce costs by over $1000 per synchrotron visit. As well as reducing travel costs, remote access allows all researchers in a group to collect their own data and, more importantly, to receive prompt feedback from other, possibly more experienced, group members. Finally, it is possible to calculate the impact of reduced travel on a beamline's carbon footprint. For ALS Beamline 4.2.2 operated by the Molecular Biology Consortium, at which almost all data is collected remotely or by local beamline staff, the carbon savings have been estimated to be 300 tons annually. ■

## Beamline 11.0.2

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microscopy experiments on stepped-platinum single-crystal surfaces revealed that the platinum surfaces undergo extensive and reversible restructuring when exposed to CO at pressures above 0.1 Torr. The study was led by M. Salmeron and G. Somorjai (both of Berkeley Lab and UC Berkeley). Stepped-platinum surfaces are viewed as models of real catalysts, which consist of small metal particles exposing a large number of low-coordination sites. The experiments revealed that as the CO surface coverage approaches 100%, the originally flat terraces of (557)- and (332)-oriented platinum crystals break up into nanometer-sized clusters. This restructuring is reversible upon pumping out the CO gas. The occurrence of large-scale surface restructuring of stepped-platinum crystals underscores the strong connection between coverage of reactant molecules and the atomic structure of the catalyst surface under reaction conditions. These results have important implications for heterogeneous catalysis where high pressures and high coverage of reactant molecules on the catalyst surfaces are the norm. ■

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### ALSNews
Subscribe to our monthly newsletter at **www.als.lbl.gov**.

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### facebook
Become a fan of the **Advanced Light Source** and get current news and events.

### ALS Web Site
Find user information, news, and science highlights at our recently redesigned Web site at **www.als.lbl.gov**.

### YouTube
Watch ALS videos, science glossaries, and more on the **AdvancedLightSource** channel.

### twitter
Follow **@ALSBerkeleyLab** to receive brief ALS updates.

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ALS ADVANCED LIGHT SOURCE

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