ALS SPECTRUM

Advanced Light Source :: Facility Report :: 2011-2012

PUBLISHED BY THE ADVANCED LIGHT SOURCE COMMUNICATIONS GROUP, AUGUST 2012

What's Inside:

U.S. DEPARTMENT OF ENERGY Office of Science

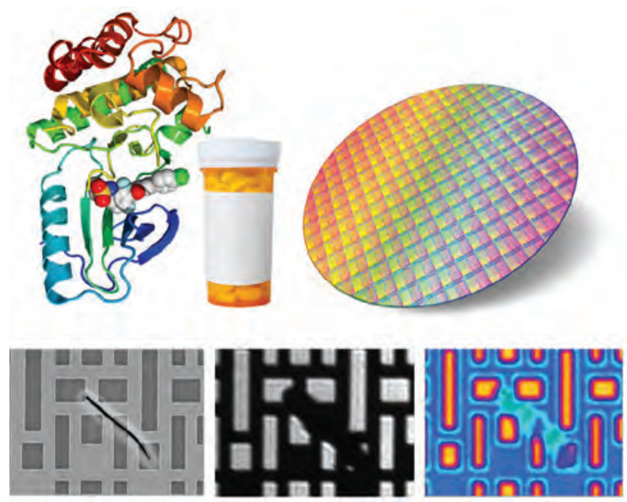
BERKELEY LAB

ALS ADVANCED LIGHT SOURCE

ALS COMMUNICATIONS

Industry at the ALS

by Sue Bailey, Corie Ralston, and Ken Goldberg



The pharmaceutical and semiconductor industries recognize the benefits of and invest significantly in synchrotron-based research. Protein structures solved using x-ray crystallography have been key to developing more effective cancer treatments, and extreme ultraviolet light has led to breakthroughs in the production of smaller, more defect-free electronic circuits.

Every year, the ALS hosts a growing, global spectrum of industrial users from a diverse set of fields. These users benefit from the ALS's outstanding technical tools, expertise, and analytical support for a wide variety of research topics. Access may be either nonproprietary (results are published openly) or proprietary, in which case a full-cost recovery charge is made for the beam time. The majority of industrial users at ALS fall into two categories: semiconductor industry researchers seeking new materials and processes for the manufacture of computer devices, and pharmaceutical or biotechnology companies that determine the structures of protein molecules to enable structure-based drug design. In both cases, the industrial users require extensive access to the

continued on page 12

Introducing Omar Yaghi, Molecular Foundry Director

by Keri Troutman

Omar Yaghi

Berkeley Lab's Molecular Foundry began with a dream of bringing together scientists who are so talented that the world wants to work with them. That vision continues with the recent appointment of renowned chemist Omar Yaghi as the Foundry's director.

Consistently ranked as one of the top scientists in the world, Yaghi is best known for his research on hydrogen and methane (natural gas) storage and his groundbreaking invention of metal-organic frameworks (MOFs), which are sometimes described as crystal sponges that can efficiently store gases. MOFs

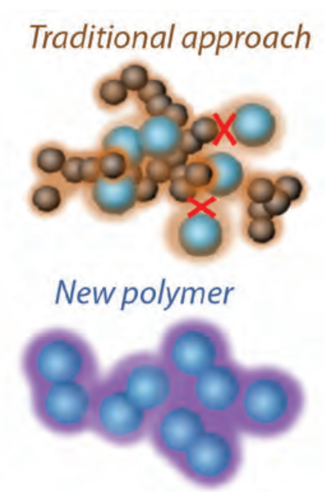
continued on page 13

Science Roundup

A Better Anode Design to Improve Lithium-Ion Batteries

Liu et al., *Adv. Mater.* **23**, 4679 (2011)

Lithium-ion batteries are in smart phones, laptops, most other consumer electronics, and the newest electric cars. Good as these batteries are, the need for energy storage in batteries is surpassing current technologies. In a lithium-ion battery, charge moves from the cathode to the anode, a critical component for storing energy. With information obtained at Beamline 8.0.1, a team of Berkeley Lab scientists has designed a new kind of anode that absorbs eight times the lithium of current designs, and has maintained its greatly increased energy capacity after more than a year of testing and many hundreds of charge-discharge cycles.

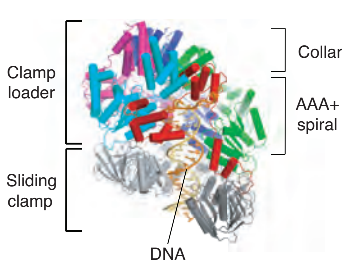


Silicon (blue) swells and shrinks while acquiring and releasing lithium ions, breaking contacts among the conducting carbon particles (brown). The new polymer (purple) is itself conductive and continues to bind tightly despite repeated swelling and shrinking.

Structures of Clamp-Loader Complexes are Key to DNA Replication

Kelch et al., *Science* **334**, 1675 (2011)

DNA replication occurs when the enzyme, DNA polymerase, moves along DNA strands at high speed, copying nucleotides as it goes. A separate ring-shaped protein complex, called the sliding clamp, attaches the polymerase to the DNA with the help of a molecular machine, the clamp loader, whose action depends on ATP. How the clamp loader accomplishes this task was unknown until researchers solved the structures of the clamp loader bound to the sliding clamp, DNA, and an ATP analog. The structures, obtained at Beamlines 8.2.1 and 8.2.2, reveal key insights into the mechanism by which the sliding clamp that facilitates replication of chromosomes is loaded onto DNA.

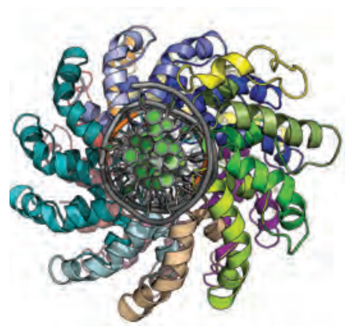


The structure of the clamp loader bound to an open sliding clamp and primer template DNA. The AAA+ modules form a symmetric, right-handed spiral that wraps around the DNA and holds the sliding clamp into an open lock-washer shape.

Genome Engineering with TAL Effector Nucleases

Mak et al., *Science* **335**,716 (2012)

Genome engineering, an emerging discipline in which a DNA sequence is altered at a single position, has a wide variety of potential uses, such as the correction of gene sequences in patients suffering from genetic diseases, the modification or insertion of genes in plants, and the generation of unique cell lines for treatment of diseases such as cancer. It requires the development of molecular tools that can search out and bind to one unique site within a complex genome while avoiding other interactions across the billions of DNA bases in a cell's nucleus. Using Beamline 5.0.2, researchers have solved the structure of one such tool called a TAL protein, learning its mechanism of action for DNA recognition and binding.

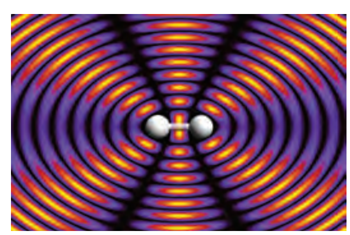


Top-down view of the structure of the DNA binding region of the TAL effector nuclease, PthXo1, in complex with its target site.

A Microscopic Double-Slit Experiment

Canton et al., *Proc. Natl. Acad. Sci.* **108**, 7302 (2011)

Two centuries ago, Thomas Young performed the classic demonstration of the wave nature of light. Along with later studies using particles instead of light, the experiment played a crucial role in establishing the validity of wave–particle duality, a puzzling concept that has ultimately become central to the interpretation of complementarity in quantum mechnanics. In a new twist on this classic experiment, the double slit (with light waves) has been replaced by a diatomic molecule (with electron waves). At Beamline 10.0.1, researchers have shown that diatomic molecules can serve as two-center emitters of electron waves and that traces of electron-wave interference can be directly observed in precise measurements of vibrationally resolved photoionization spectra.



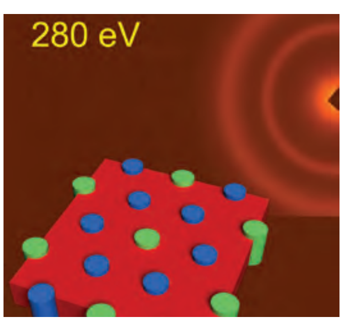
Depiction of electron waves interfering with each other as they propagate outward from a diatomic molecule. Rendered by Etienne Plésiat.

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

Resonant Soft X-Ray Scattering of Tri-Block Copolymers

Wang et al., *Nano Lett.* **11**, 39061 (2011)

In principle, tri-block copolymers, consisting of three chemically distinct polymers covalently joined together at the ends of each polymer chain, can serve as scaffolds and templates for fabricating a vast number of nanostructures. An international team has succeeded in combining resonant soft x-ray scattering (RSoXS) at Beamline 11.0.1 with transmission electron microscopy tomography and other techniques to unambiguously determine morphologies comprising two nested hexagonally packed arrays of nanoscopic, cylindrical microdomains in the bulk and a core-shell nanostructure in a thin film. Not only has this work revealed a new phase of tri-block copolymer with complicated morphology, it has illustrated the importance of RSoXS as a unique, powerful tool for examining complex, multi-component systems.

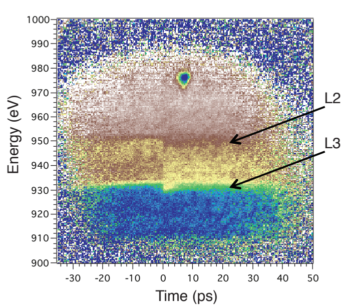


Schematic illustration of hexagonally packed cylindrical morphology of the IS2VP tri-block copolymer. At upper right, the RSoXS pattern at 280 eV shows contributions from all three polymers (red, green, and blue).

Ultrafast Spectroscopy of Warm Dense Matter

Cho et al., *Phys. Rev. Lett.* **106**, 167601 (2011)

Being neither solid, liquid, gas, nor plasma, warm dense matter (WDM) occupies a no man's land in the map of material phases. Its temperature can range between that of planetary cores to that of stellar cores. Not only is it prevalent throughout the universe, it is relevant to inertial confinement fusion and material performance under extreme conditions. However, because of its extreme temperatures and pressures, WDM tends to be drastically transient and thus difficult to study in the laboratory. Now, researchers have set up ultrafast x-ray absorption spectroscopy at Beamline 6.0.2 to measure the electronic structure of WDMs, demonstrating that fast-changing electron temperatures of matter under extreme conditions can be determined with picosecond resolution.

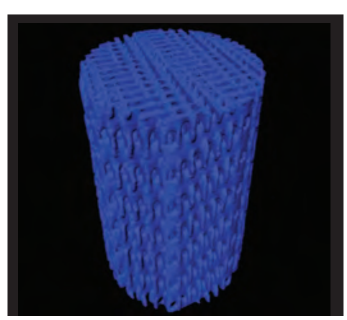


Warm dense copper was created by a femtosecond laser and probed. The broadband spectrum was swept across the CCD detector of an x-ray streak camera for picosecond temporal resolution.

Bioactive Glass Scaffolds for Bone Regeneration

Fu et al., *Acta Biomater.* **7**, 3547 (2011)

Natural materials are renowned for their unique combination of outstanding mechanical properties and exquisite microstructure. For example, bone, cork, and wood are porous biological materials with high specific stiffness (stiffness per unit weight) and specific strength. The outstanding mechanical properties of these materials are attributed to their anisotropic structures, which have optimized strength-to-density and stiffness-to-density ratios. Working at ALS Beamline 8.3.2, researchers have created bio-active glass scaffolds that mirror nature's efficient materials. The three-dimensional glass scaffold is as porous as trabecular bone, has a compressive strength comparable to that of cortical bone, and has a strength-to-porosity ratio higher than any previously reported scaffolds.

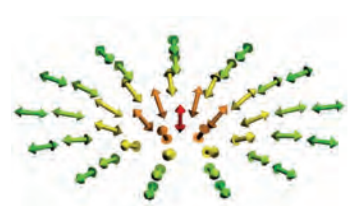


A three-dimensional visualization of the sintered 6P53B glass scaffolds using synchrotron x-ray microcomputed tomography.

Direct Imaging of Antiferromagnetic Vortex States

Wu et al., *Nat. Phys.* **7**, 303 (2011)

Magnetic materials are characterized by the ordering of electron spins, with nearest-neighbor spins parallel to each other in ferromagnetic (FM) materials and antiparallel in antiferromagnetic (AFM) materials. As the size is reduced to micron scale, the spins in an FM microstructure can curl around to form a magnetic vortex state. There has been no direct observation of such states in an AFM microstructure, although theory predicts many interesting properties. A research team now has taken the first direct image of an AFM vortex in multilayered magnetic disk structures using x-ray magnetic linear dichroism and photoemission electron microscopy at Beamlines 4.0.2 and 11.0.1, respectively. The experiments observed two types of AFM vortices, one of which has no analogue in FM vortices.



A divergent vortex structure was observed in thicker AFM films. This type of divergent vortex is never allowed in FM microstructures because it would result in a net magnetic charge at the disk boundary.

continued on page 24

THE RING **AROUND THE RING** AROUND THE RING AROUND THE

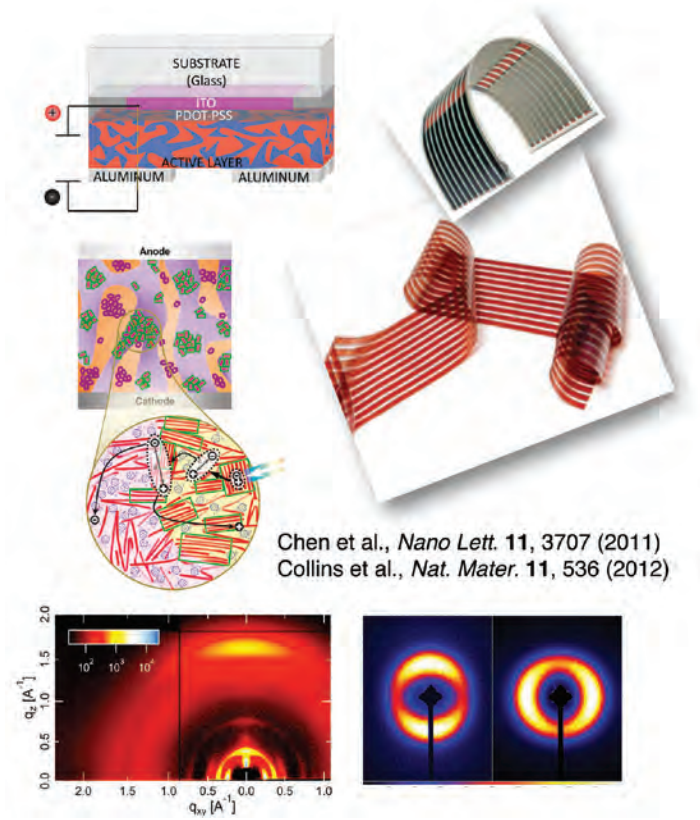
EXPERIMENTAL SYSTEMS GROUP: ENERGY RESEARCH

by Howard Padmore and Cheng Wang

As part of the global revolution in renewable and carbon-neutral energy technologies, the Experimental Systems Group (ESG) at the ALS has been an active player in developing and applying the techniques of synchrotron radiation to research in this area. With the development of powerful detectors and advanced computation in combination with the brilliant x-ray source of the ALS, ESG is operating a suite of world-class x-ray tools that are widely used for exploring the mesocale, electronic, and atomic structure of materials. These tools include small- and wide-angle x-ray scattering (SAXS/WAXS), x-ray tomography, chemical crystallography, high-pressure diffraction, microdiffraction, photoemmission electron microscopy (PEEM), micro x-ray absorption spectroscopy, and ultrafast x-ray spectroscopy.

In addition, the ESG is a leader in developing new research tools such as resonant soft x-ray scattering (R-SoXS) and coherent diffraction microscopy (COSMIC), with the goal of better characterization of the chemical and physical properties of matter that will aid the design and production of better materials for sustainable energy needs.

In combination with our user community, the group collaborates and works on many areas in energy research, including energy generation using sustainable sources such as solar energy harvesting (organic photovoltaics studied with x-ray scattering), biofuels (collaborating with the Joint BioEnergy Institute on x-ray tomography), fundamental study of the structure of materials used for nuclear fusion (microdiffraction experiment on deuterium and tritium capsules), the development of efficient energy conversion based on artificial photosynthesis (Joint Center for Artificial Photosynthesis research using x-ray scattering), fuel cells (structural characterization with x-ray scattering, microdiffraction), lithium-ion batteries (x-ray scattering, x-ray absorption spectroscopy, microdiffraction), low power-consumption computational elements (PEEM3), smart catalysts that will greatly reduce energy consumption (small-molecule crystallography), the study of new materials to be used for building safer nuclear power plants (microdiffraction), and carbon capture and storage (x-ray tomography). Here we give a few examples of this collaborative work.



X-ray scattering methods have recently been widely used as high-resolution, nondestructive probes for characterizing mesoscale structure in organic photovoltaics (OPVs). They provide the ability to determine how organic electronic materials organize on small length scales during device fabrication and how that translates into their operation in an OPV device.

Polymer Solar Cells with Hard and Soft X-Ray Scattering: From Hierachical Structure to Local Molecular Ordering. Solar electricity remains one of the most promising forms of alternative energy. The development of solution-processable organic electronic materials has enabled the use of low-cost deposition methods such as roll-to-roll printing to make organic solar cells. World-record organic solar cells have efficiencies of more than 10% and are now reaching commercial viability. Organic photovoltaics (OPVs) are particularly appealing as low-cost and scalable options because they are composed of less-expensive materials and have simpler processing requirements. X-ray scattering methods have recently been widely used as high-resolution, nondestructive probes for characterizing mesoscale structure in OPVs. The scattering represents a statistical average over a large sample area and therefore offers a great complement to direct-imaging techniques such as electron microscopy and scanning probe microscopy. X-ray scattering is the only research tool that allows high-throughput and dynamic in situ characterization. It provides the ability to determine the fundamental connection between how organic electronic materials organize on small length scales during device fabrication and how that translates into their operation in an OPV device.

Researchers have performed hard and soft x-ray scattering on PTB7/fullerene bulk heterojunction (BHJ) solar

continued on page 5

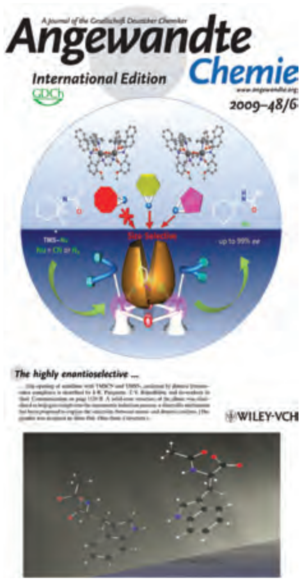
THE RING AROUND THE RING AROUND THE RING AROUND THE

ESG: Energy Research

continued from page 4

cells at Beamlines 7.3.3 and 11.0.1 to probe performance-related structures at different length scales. This class of solar cell material currently holds a world record conversion efficiency (>10%). The active layers were initially thought to consist of an interpenetrating network of pure polymer (PTB7) domains and pure fullerene domains, separated by discrete interfaces. However, x-ray scattering demonstrated that the superior performance of PTB7/fullerene solar cells is attributed to surprising hierarchical nanomorphologies ranging from several nanometers of crystallites to tens of nanometers of nanocrystallite aggregates in intermixed PTB7-rich and fullerene-rich domains, themselves hundreds of nanometers in size. Furthermore, a new resonant x-ray scattering method using polarized soft x-rays was developed and demonstrated at Beamline 11.0.1. The scattering technique reveals molecular alignment independent of crystallinity and represents an important new tool for examining the connection between electron transport properties and morphology. This work has revealed the impact of the orientation of polymer chains on charge-carrier mobility and uncovered the organization of polymer domains in blends used for solar cells. These correlations are valuable for a better understanding of charge generation at polymer–polymer interfaces in solar cells, guide better molecular design, and ultimately improve the performance and commercial viability of this novel technology.

Small Molecular Crystallography on Enantioselective Catalysts: One Hand Produces Less Waste and Need for Separation. Like humans, molecules (chiral compounds) can come in both left- and right-handed forms, which are called enantiomers. They are mirror images of each other as a right hand is of the left. An enantiomer's handedness is determined by the direction to which they rotate light. What makes a lemon smell like a lemon and an orange like an orange is in fact the same molecule, limonene, but with different handedness. The smell receptor is shape selective and responds differently to the two versions. The same is true for sugar: both enantiomers taste sweet but only one can fuel the human body. Life itself is based on amino acids, which are chiral compounds. However, living systems favor the left-handed forms and so proteins are predominantly left-handed. As a result, when proteins and enzymes are formed, their active sites are shape-selective to only accept one enantiomer and ignore the other, and the product of the reaction in itself is chiral.



Small-molecule crytallography at Beamline 11.3.1 has helped elucidate why certain catalysts are more effective than others at producing molecules with the desired chirality. Learning from nature and using "shape selection" in chemical reactions and drug synthesis could result in less waste and energy used for separations in the chemical and pharmaceutical industries.

The chemical industry and specifically the pharmaceutical industry, where now 80% of production is of chiral compounds, need to produce compounds with the correct handedness. If none of the starting materials are chiral (have no handedness), then the product is a 50:50 mixture of both chiralities. As only one enantiomer generally has the medicinal properties required, and in some cases the other has adverse effects on the patient, they have to be separated. This separation is complicated and expensive because the two enantiomers are chemically the same, and in the end, half the material made is wasted. What is needed is to take a lesson from nature's catalysts and enzymes, and use shape selection in the reaction.

The synthesis of a drug molecule is a many-step process, and at each step there is potential for waste, either through incomplete reactions or the formation of unwanted products requiring separation. For example, one such step includes the ring opening of aziridines. A series of yttrium-based chiral catalysts have been synthesized and reacted with a series of aziridines. The most successful catalyst produced greater than 99% of the expected yield of the desired molecule and between 0.5% and 2% of the unwanted enantiomer. The crystal structure of the catalyst, determined on Beamline 11.3.1, showed how the atoms of the ligands are arranged around the yttrium atom and the shape-selective pocket where the reaction occurs. By knowing the shape of the catalyst and reaction pocket, an understanding of the reaction mechanism is possible. This leads to the rational design of new and more efficient catalysts, resulting in less waste and energy used in subsequent separations.

CO_2 Storage and Capture: Insights from X-Ray Diffraction and Tomography. Capturing and storing CO_2 emissions could prevent the carbon cycle disruption caused by burning fuels. While coal and natural gas are plentiful and inexpensive fuels for energy production, the combustion of these fuels to create electricity is the single largest source of greenhouse-gas emissions in the United States, accounting for over 40% of all CO_2 emissions. Researchers are seeking workable ways to capture and sequester the CO_2 produced by these power plants.

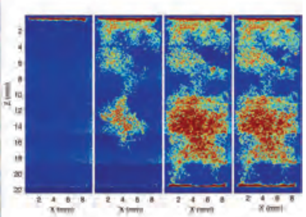
Metal organic frameworks (MOFs) are promising, nanoporous materials whose pore sizes and internal surface chemistry can be tailored to selectively trap CO_2 molecules, allowing nitrogen, oxygen, and other non-greenhouse gases to return to the atmosphere.

continued on page 6

RING AROUND THE RING AROUND THE RING AROUND THE RING **AROUND THE RING**

ESG: Energy Research

continued from page 5



X-ray diffraction can precisely locate the gas species trapped inside metal organic frameworks, which are nanoporous molecules that show promise for selectively capturing CO_2. X-ray microtomography reveals the flow properties of CO_2 when injected into underground rock structures.

Single-crystal hard x-ray diffraction at Beamline 11.3.1 was used to precisely locate the gas species trapped inside MOFs. The crystal structure information has provided theorists with critical data needed to validate models aimed at describing and predicting the performance of MOFs in CO_2 capture scenarios.

Once captured, the carbon dioxide will have to be stored for the long term. Geoscientists at Berkeley Lab are exploring all facets of long-term geological storage of carbon dioxide, including the interaction of CO_2 with the various minerals and microbes found deep underground. When injected into underground rock structures, the flow properties of CO_2 are dominated by the innumerable fluid/fluid exchange interactions within the micron-sized pores of the rock. Understanding these interactions is the key to predicting the behavior of underground CO_2 reservoirs. Using synchrotron light, we are able to look inside rocks with three-dimensional x-ray microtomography at Beamline 8.3.2 to see how fluids flow through permeable rock, displacing existing liquids. These experiments yield the data that will confirm the theoretical models being developed that will in turn be used to predict the properties of large CO_2 underground reservoirs.

SCIENTIFIC SUPPORT GROUP: MAESTRO, MATERIALS, AND MENTORING

by Zahid Hussain, Mike Martin, and Eli Rotenberg

The Scientific Support Group (SSG), in addition to providing scientific and technical support to ALS users, strives to create state-of-the-art instrumentation to enable new science.

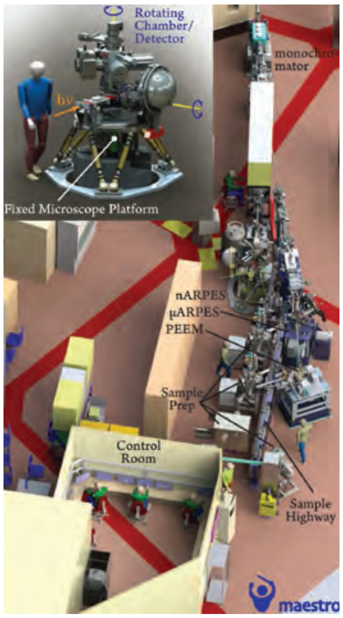
A New Era in ARPES at Beamline 7: MAESTRO. October 2012 marks a milestone in the angle-resolved photoemission spectroscopy (ARPES) program at Sector 7 of the ALS. After 19 years of continuous operation, Beamline 7.0.1 will be closed down for a complete renovation in which the entire facility will be replaced from the insertion device to the endstations. The new facility, dubbed "MAESTRO" (Microscopic and Electronic Structure Observatory), is scheduled to be commissioned in 2013 and will derive its light from a full-variable-polarization (linear and circular) insertion device coupled to an entrance-slitless, variable-line-space plane-grating monochrometer with 10 times better energy resolution (3 meV at 100 eV) than the old beamline. It will also feature endstations that will be capable of ARPES in three outstanding modes:

- The new microARPES (μARPES) chamber, a refurbished version of the existing "Electronic Structure Factory" endstation, will feature a spot size five times smaller (< 10 μm) than the previous version.
- The new nanoARPES (nARPES) chamber will feature a spatial resolution 1000 times better (down to 50 nm) and an energy resolution 2.5 times better (down to 10 meV) than the previous ARPES capabilities.
- A new photoemission electron microscope (PEEM) for ARPES, reaching moderate spatial resolution (< 2 μm) as well as moderate energy resolution (< 200 meV) and angle resolution (1°), will also be available. This ARPES capability will be combined with full-field real-time imaging of structure and chemical mapping of surfaces. With a built-in small-spot He I resonance lamp, it will be an important aid to the off-line growth and selection of samples. With access to soft x-rays from the beamline, it will also serve as a fully capable ARPES endstation in its own right, augmenting the other PEEMs at the ALS with an emphasis on electronic band structure determination of in-situ grown samples and correlated materials.

The existing suite of in situ sample-preparation capabilities, including sputter/annealing and thin-film growth by both molecular-beam epitaxy (MBE) and pulsed-laser deposition (PLD), will be preserved, and a new capability for four-probe microtransport measurements will be added. Chambers for all of these functions are connected to the experimental endstations by a continuous "sample highway" that can share all samples among all three endstations without

continued on page 7

SSG: Maestro *continued from page 6*



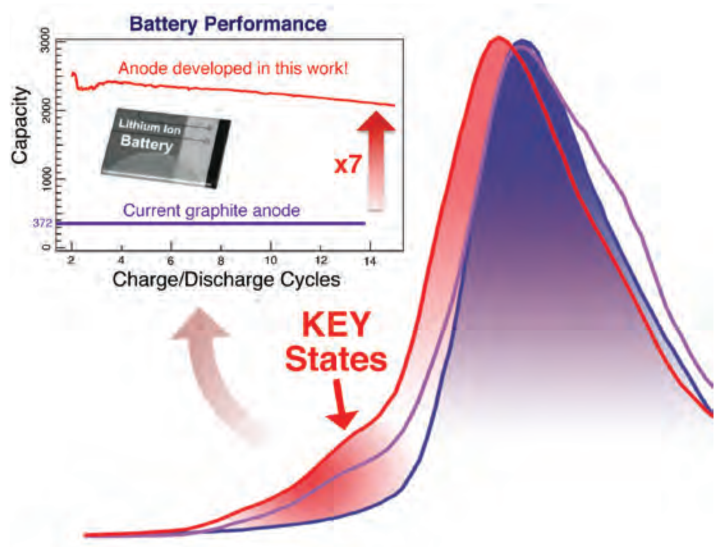
Rendering of MAESTRO beamline currently planned for commissioning at ALS Sector 7 after demolition of the old beamline in the fall of 2012. It consists of nanoARPES, microARPES, and PEEM endstations, which share samples with multiple preparation chambers through an ultrahigh-vacuum sample highway. Inset: The nanoARPES chamber conceptual design.

removal from the ultrahigh-vacuum environment.

The most novel feature of the beamline will be the new nARPES chamber. This instrument works by focusing the incoming x-ray beam onto samples that are mounted onto a high-precision ultrahigh-vacuum scanning stage. A focus down to 50 nm is obtained by passing the x-rays through a Fresnel zone plate followed by an order-sorting aperture.

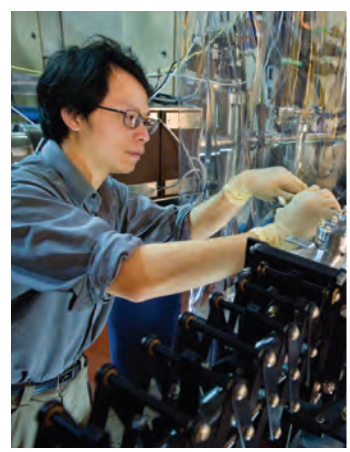
High spatial resolution means that there are demanding requirements on photon flux and sample stability. In designing the nARPES chamber, great effort was expended to meet these demands without sacrificing flexibility. The endstation will be capable of sampling photoemitted electrons at a very wide range of angles, including emission perpendicular to the sample surface. This is achieved by employing a special microfabricated order-sorting aperture that is designed to occlude the smallest possible amount of photoelectrons emitted from the sample. In addition, a special vacuum chamber was constructed that allows the Scienta R4000 electron analyzer to rotate in two angles about the fixed microscope. This will allow access to a "phase space" of electron emission comparable to that which can be achieved in today's ordinary ARPES chambers.

Developing Materials for High-Performance Lithium Ion Batteries. Improvements in the capacity and safety of lithium-ion batteries have become more and more critical to realizing the potential of plug-in electric vehicles with longer driving ranges. Materials with high lithium storage capacity, such as silicon and tin, have long been reported. However, in practice, they suffer from a severe volume-change problem that degrades their performance over time. Now, a collaboration involving material synthesis, soft x-ray spectroscopy, and theoretical simulation has established a novel approach for developing a polymer material that can maintain both the mechanical and electrical integrity of the electrode, leading to the best cycling performance so far of composite anodes without the need for conductive additives. Soft x-ray spectra collected at Beamline 8.0.1 reveal directly the key electronic states associated with a particular functional group that is critical for the greatly improved battery performance. [Liu et al., *Adv. Mater.* **23**, 4679 (2011).]



Critical electronic states, as revealed by soft x-ray spectroscopy, correspond to a particular component of the material and a great improvement in battery performance. Such information provides unambiguous guidelines for material development and optimization

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



Yi-De Chuang

Awards and Honors. SSG member Yi-De Chuang recently received the prestigious Klaus Halbach Award for innovative instrumentation at the ALS. The award cited his work on "Time-resolved and conventional resonant soft x-ray scattering (RSXS) spectroscopy for

continued on page 17

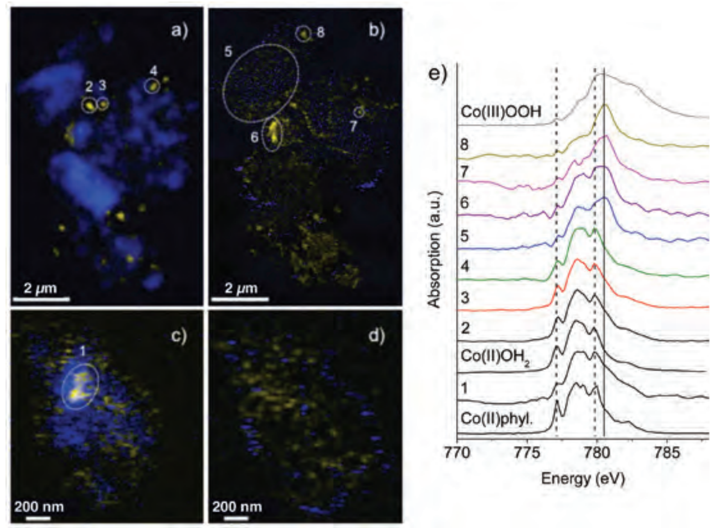
RING AROUND THE RING AROUND THE RING AROUND THE RING AROUND THE RING

MOLECULAR ENVIRONMENTAL SCIENCE AT BEAMLINE 11.0.2

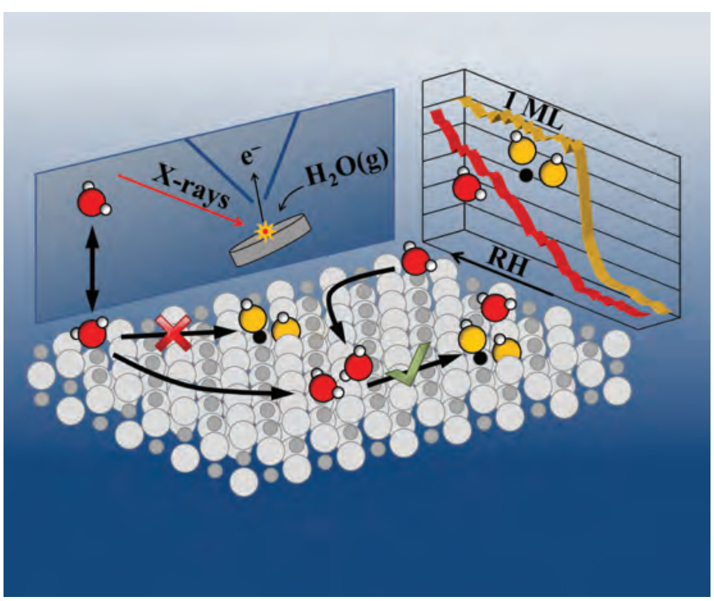
by Hendrik Bluhm, Mary K. Gilles, David K. Shuh, and Tolek Tyliszczak

Beamline 11.0.2 continues to be productive scientifically while technical advancements for existing and new endstations proceed. Scanning transmission x-ray microscopy (STXM) experiments here look at soils, catalysts, star dust, actinides, energy, atmospheric aerosols, and the magnetic properties of materials. Experiments at the ambient-pressure photoemission spectroscopy (APPES) endstation focus on environmental science, catalysis, and energy science.

Cement-based materials play an important role in multi-barrier concepts for the disposal of low- and intermediate-level radioactive wastes. Cobalt is an important contaminant in waste materials generated in medical applications and industrial processes. Thus, molecular-level information on the speciation of Co in cement is desirable for a more detailed assessment of its leachability from landfills and contaminated soils into aquifers. STXM and NEXAFS were used to investigate the speciation and spatial distribution of Co in a Co(II)-doped cement matrix. Based on the shape of the absorption spectra, it was found that Co(II) was partly oxidized to Co(III). Its correlation and anticorrelation with elements such as Al, Si, and Mn show that Co(II) is predominately present as a Co-hydroxide-like phase as well as Co-phyllosilicate, whereas Co(III) tends to be incorporated only into a CoOOH-like phase. The study thus suggests that Co(III)-containing phases should be considered as solubility-limiting phases with respect to Co release from Co-containing cementitious waste repositories under oxidizing conditions [Dähn et al., *Environ. Sci. Technol.* **45**, 2021 (2011)].



Left: STXM elemental distribution maps of Co(II)-doped cement particles. Right: NEXAFS spectra collected from different regions (a-d) indicated by numbers 1-8 together with spectra of reference compounds [Co(II) phyllosilicate, Co(II)OH$_2$ and Co(III)OOH]. Energy positions for the vertical lines are 777.1, 779.85, and 780.5 eV, indicating where the maps were collected.



Suggested mechanism for the autocatalytic dissociation of water on MgO(100), which proceeds through the formation of complexes involving several water molecules and surface oxygen.

Understanding the interaction of water with metal oxides has implications in environmental chemistry, materials science, and catalysis. Despite the importance of water on metal oxide surfaces in a wide array of fields, relatively little is known about the interfacial chemistry of water vapor in equilibrium with metal oxide surfaces under ambient conditions of temperature and relative humidity. Recently a team of researchers from Berkeley Lab and Stanford University used ambient-pressure XPS at Beamline 11.0.2 to investigate the dissociation of water on magnesium oxide films as a function of relative humidity (RH). Under low RH conditions (RH < 0.01%), water dissociates only at defect sites, whereas at higher RH values (RH > 0.01 %), water autocatalytically dissociates at flat terrace sites. At 20% RH, there exists ~1 monolayer of water at the surface interacting with a fully hydroxylated interface [Newberg et al., *J. Phys. Chem. C* **115**, 12864 (2011)].

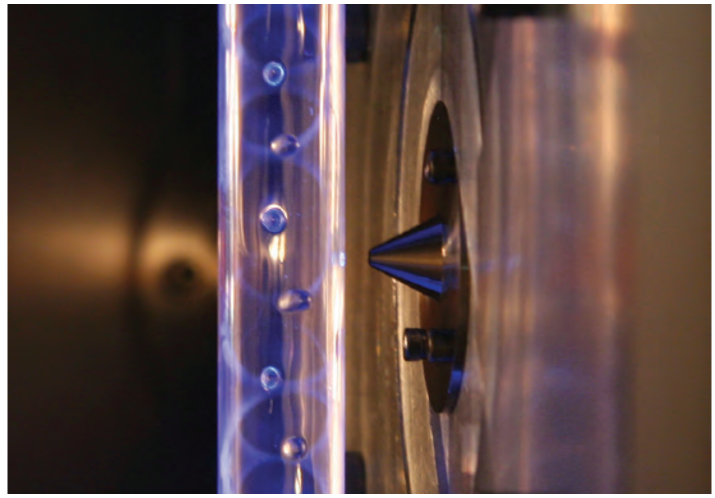
CHEMICAL DYNAMICS: FOUR HIGHLIGHTS

by Musa Ahmed

Cappa and Wilson, *Atmos. Chem. Phys.* 11, 1895 (2011). Most global climate and air-quality atmospheric models assume that organic aerosols (OA) are liquids in equilibrium with the surrounding atmosphere. However, recent work has suggested that OA may exist in the atmosphere as "glasses," having large implications for how to represent the atmospheric chemistry of organic aerosols in computer models. Cappa and Wilson used vacuum ultraviolet (VUV) photoionization aerosol mass spectrometry at the Chemical Dynamics Beamline (9.0.2) to measure the evolution of the chemical composition of two large classes of OA. Differences in the VUV mass spectra for different temperatures and aerosol types were observed. It was postulated that the difference arises because the diffusivity within certain particles is slow enough that they do not exhibit the expected liquid-like behavior and perhaps exist in a glassy state. To reconcile these observations with decades of aerosol growth measurements that indicate that OA formation is described by equilibrium partitioning, Cappa and Wilson presented a conceptual model wherein an OA can be formed and then rapidly converted from an absorbing form to a non-absorbing form. The results suggest that, although OA growth may be described by equilibrium partitioning theory, the properties of the OA once formed may differ significantly from the properties determined in the equilibrium framework.

Soorkia et al., *Rev. Sci. Instrum.* 82, 124102 (2011). Wilson, Leone, and co-workers developed a new pulsed Laval nozzle apparatus with VUV synchrotron photoionization quadrupole mass spectrometry to study low-temperature radical-neutral chemical reactions of importance for modeling the atmosphere of Saturn's moon, Titan, as well as the outer planets. A design for the sampling geometry of a pulsed Laval nozzle expansion has been developed that successfully determines rate coefficients by time-resolved mass spectrometry. The new concept employs airfoil sampling of the collimated expansion with excellent sampling throughput. The reaction of C_2H with C_2H_2 was studied at 70 K as a proof-of-principle result for both low-temperature rate coefficient measurements and product identification based on the photoionization spectrum of the reaction product versus VUV photon energy.

Welz et al., *Science* 335, 204 (2012). Ozonolysis is a major tropospheric removal mechanism for unsaturated hydrocarbons and proceeds via "Criegee intermediates"—carbonyl oxides—that play a key role in tropospheric oxidation models. However, until recently no gas-phase Criegee intermediate had been observed, and indirect determinations of their reaction kinetics gave derived rate coefficients spanning orders of magnitude. At Beamline 9.0.1, Taatjes and co-workers report direct photoionization mass spectrometric detection of formaldehyde oxide (CH_2OO) as a product of the reaction of CH_2I with O_2. This reaction enabled direct laboratory determinations of CH_2OO kinetics. Upper limits were extracted for reaction-rate coefficients with NO and H_2O. The CH_2OO reactions with SO_2 and NO_2 proved unexpectedly rapid and imply a substantially greater role of carbonyl oxides in models of tropospheric sulfate and nitrate chemistry than previously assumed.



The chemical reactions of Criegee intermediates were studied using an apparatus at Beamline 9.0.2. A quartz reaction tube shows the faint blue luminescence from a 248-nm laser that creates a precursor reactant. A gas beam of the reactants and products exits the tube through a 600-µm pinhole facing the conical skimmer on the right, which collects the molecules for eventual ionization by vacuum ultraviolet photons from the ALS and detection by a mass spectrometer. Photo by David Osborn (Sandia National Laboratories).

Golan et al., *Nat. Chem.* 4, 323 (2012). Proton transfer is ubiquitous in chemistry and biology, occurring, for example, in proteins, enzyme reactions, and across proton channels and pumps. However, it has always been described in the context of hydrogen-bonding networks ("proton wires") acting as proton conduits. At Beamline 9.0.1, using molecular beams and photoionization mass spectrometry coupled to state-of-the-art electronic structure calculations, efficient intramolecular ionization-induced proton transfer across a 1,3-dimethyluracil dimer, a model π-stacked system with no hydrogen bonds was reported. Upon photoionization by tunable vacuum ultraviolet synchrotron radiation, the dimethyluracil dimer undergoes proton transfer and dissociates to produce a protonated monomer. Deuterated dimethyluracil experiments confirm that proton transfer occurs from the methyl groups and not from the aromatic C–H sites.

CXRO: PUSHING THE BOUNDARIES IN OPTICS AND IMAGING

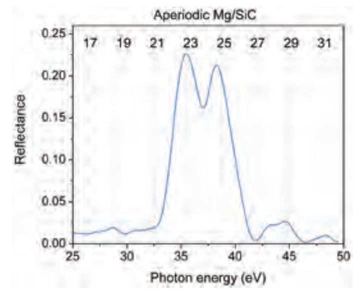
by Patrick Naulleau

The tight collaboration between the Center for X-Ray Optics (CXRO) and the ALS has continued to bear fruit this past year. Industrially funded activities in the extreme ultraviolet (EUV) lithography domain have expanded and major new initiatives kicked off. We are looking forward to bringing these projects to fruition in the near future.

In the past year CXRO has continued to push the boundaries in x-ray/EUV optics and imaging. One of our biggest advancements in the nanofabrication area has been the development of a robust process for fabricating free-standing zone plates. These devices enable significant improvements in throughput and are less susceptible to contamination. For our EUV applications, we have seen improvement in efficiency by a factor of two compared to conventional zone plates.

The CXRO focus in the area of optics coatings remains on aperiodic structures with engineered functionality, such as increased or reduced bandwidth and temporal pulse chirping. For some applications, it is desirable to utilize more than one harmonic from a high-harmonic source. However, the bandwidth of a high-reflectivity Mg/SiC multilayer is typically only wide enough to reflect a single harmonic. While it is possible to increase the multilayer bandwidth by

Free-standing EUV zone plate with pseudo-random support structures for minimized impact on imaging and optimal robustness.

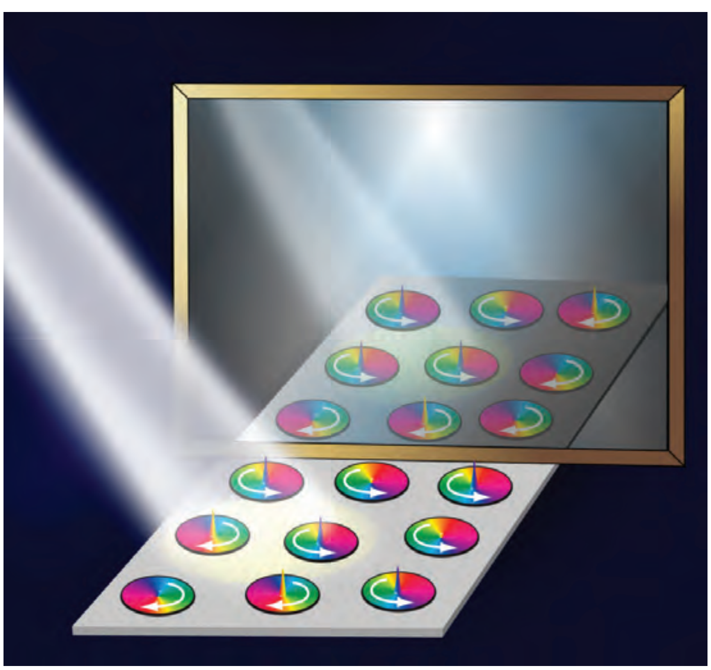


Spectral response of a recently fabricated harmonic-selecting mirror design for 13.5 nm, achieving 20% reflectivity while strongly suppressing even the nearest-neighbor harmonics.

reducing the number of periods, this comes at the cost of reduced reflectivity. By using an aperiodic design, a Mg/SiC multilayer mirror was fabricated to reflect two adjacent harmonics with a reflectivity in the range of 20% for the 23rd and 25th harmonics (fundamental wavelength is 800 nm). The high-accuracy measurements were performed at Beamlime 6.3.1.

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: elemental, chemical, topological, and magnetic. As part of the magnetic materials program within Berkeley Lab's Materials Sciences Division, the nanomagnetism research using XM-1 is focused on a fundamental understanding of magnetic properties down to fundamental length and time scales. In addition to being the cornerstone of CXRO's nanomagnetism research, XM-1 also continues to support a vibrant ALS user program including activities beyond nanomagnetism. On the instrument side, the past year has seen great progress in the implementation of tomographic capabilities at XM-1. Additionally, progress has been made in working with environmental cells to study effects such as catalysis. Our nanomagnetism activities made substantial contributions to understanding complexity, functionality, and stochastic behavior—characteristics of mesoscale phenomena. The most important achievement was the finding that the nucleation process of magnetic vortices shows a significant asymmetry, which could be explained as being caused by surface-related interactions. This effect has to be taken into account for potential future devices based on magnetic vortices.

The past year has also brought about a large expansion of CXRO's extreme ultraviolet lithography (EUVL) research program. Through this program, CXRO provides the semiconductor industry with research capabilities generations ahead of their current processes. The expansion includes increased operation of current tools and development



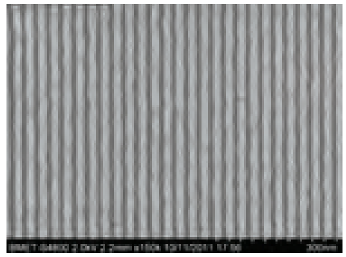
An artist's rendering of the observed breakdown in symmetry of the magnetic vortices nucleation process.

continued on page 11

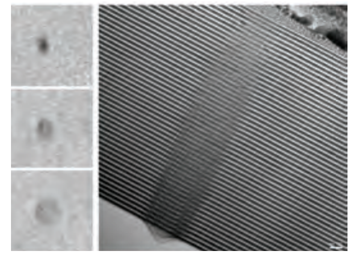
CXRO

continued from page 10

of new state-of-the-art tools. The SEMATECH Berkeley Micro Exposure Tool (MET) on Beamline 12.0.1 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 over a thousand new lithography materials being tested every year. The ability to print 16-nm lines and spaces in a new experimental photoresist with 31-mJ/cm² sensitivity represents a nearly 3x improvement in sensitivity over the past year. At the neighboring Beamline 11.3.2, the SEMATECH Berkeley Actinic Inspection Tool (AIT) is an EUV zone-plate-based full-field microscope dedicated to reflective photomask research. As the highest-performing tool of its kind, the AIT serves researchers from the leading semiconductor companies, providing fundamental learning not available anywhere else. Defects on EUV masks are one of the most crucial challenges facing the industry. Understanding how the physical characteristics of defects manifest themselves as image errors is of utmost importance. Images from our EUV microscope can show how buried, pit-like defects disrupt the local reflectivity (image intensity).



An experimental resist with 16-nm lines and spaces printed with 31-mJ/cm² sensitivity using the SEMATECH Berkeley MET at Beamline 12.0.1.3.



Two views of a defect on an EUV photomask. (Left) Top-down images from our EUV microscope show the defect disrupting the reflectivity. (Right) Cross-sectional transmission electron microscopy (TEM) through the reflective multilayer mirror coating and substrate reveals that the disturbance comes from a buried, pit-like defect.

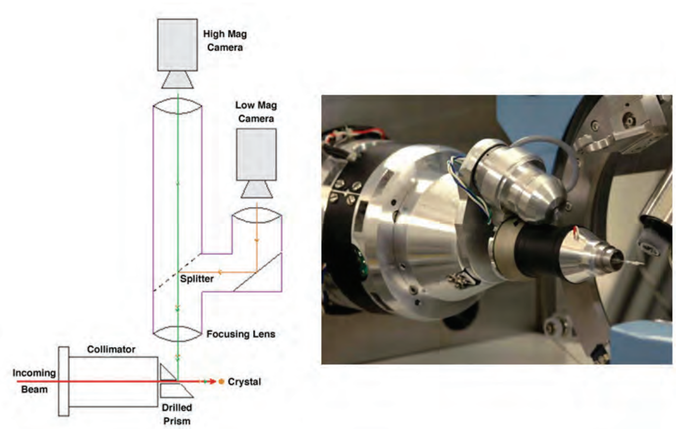
STRUCTURAL BIOLOGY: AWARD-WINNING INNOVATION

by Corie Ralston

The Berkeley Center for Structural Biology (BCSB) has seen another busy year, with several new beamline optics and endstation upgrades. Four of the five beamlines run by the BCSB now have a Compact Variable Collimator (CVC) installed. Invented by scientists in the BCSB and selected as one of the 2012 R&D100 awards, this collimator makes it possible for users to choose the exact size of the beam with ease and precision. Matching the beam to the crystal size in a crystallography experiment greatly improves the signal-to-noise ratio in data collection because it significantly reduces the background scattering from the crystal buffer and allows useful data collection on even tiny crystals. In addition, the CVC allows selected portions of a crystal to be used for data collection. In conjunction with the hardware implementation, software was developed in-house to scan crystals quickly using the CVC and automatically choose the best diffracting spot on the sample for further data collection. This has made previously unusable samples yield high-quality diffraction data, since it is now possible to selectively choose one crystal among several that were looped or grown together, or to easily pinpoint the one small, defect-free volume of the crystal.

As smaller crystal samples become more typical, sample-centering stability and viewing become much more critical. To address this need, the three

Continuous-zoom gigabit Ethernet (gigE) high-magnification camera.



Sample viewing at Beamline 5.0.2 is in-line with the x-ray beam. In conjunction with a highly stable goniometer, MiniKappa stage, and CVC, this allows centering and data collection from crystals down to 5 microns in diameter.

continued on page 12

RING AROUND THE RING AROUND THE RING AROUND THE RING **AROUND THE RING**

BCSB: Innovation *continued from page11*

wiggler beamlines run by the BCSB were installed with new viewing optics. Based on the design used in the Sector 8 minihutch macromolecular crystallography beamlines, the new viewing systems include a small mirrored prism with a through-hole, which allows the x-rays to pass through the prism, while visible light is reflected back up into a high-magnification CCD camera for live, continuous-zoom, high- resolution, in-line sample viewing.

In addition, an MD2-Lite goniometer system was installed on Beamline 8.2.2, allowing precise (2-micron sphere-of-confusion) centering. The system is similar to the MD2 already installed on Beamline 8.2.1, and another system is slated for installation on Beamline 5.0.2 later in the year. The MD2 systems include a MiniKappa option, in which the stage can be rotated off-axis for crystals with particularly long unit cells that require re-orientation in the beam. All these improvements together push the frontier in protein crystallography, allowing structure solution from crystals too small or otherwise flawed to have been useful even just five years ago.

Industry Stories *continued from page 1*

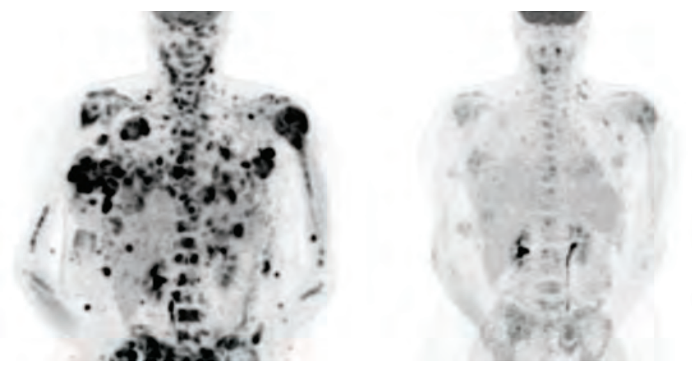
facility and have therefore established Participating Research Teams (PRTs) that invest in building, maintaining, and supporting the beamlines that they use.

The semiconductor industry obtains access to the ALS through a PRT formed jointly by SEMATECH, a research consortium of leading, global semiconductor manufacturers, and the Center for X-Ray Optics (CXRO), a research group within Berkeley Lab's Materials Sciences Division. Their research is paving the way for the use of extreme ultraviolet (EUV) lithography, an advanced method of mass-producing computer chips with ever-smaller circuit sizes, using short-wavelength light.

SEMATECH is currently focused on two research challenges at the ALS. The first is to produce defect-free EUV masks—"master" glass plates that carry layers of the printed circuit pattern. The SEMATECH Berkeley Actinic Inspection Tool (AIT) at Beamline 11.3.2 is a unique microscope established to detect and characterize all types of mask defects [Mochi et al., *Proc. SPIE* **7636**, 76361A (2010)]. The second research challenge is to develop ultrahigh-resolution photoresist materials—light-sensitive films into which the nanometer-scale circuit patterns are printed. The goal is to discover materials and processes that simultaneously support low line-edge roughness, high sensitivity, and increased resolution. The SEMATECH Berkeley Microfield Exposure Tool (MET) was created to speed research in this area. To date, lines with sizes below 16 nm, with 2-nm line-edge roughness have been achieved; this represents the highest resolution ever achieved from a single-exposure projection optical lithography tool, a significant breakthrough in single-exposure projection printing resolution [Naulleau et al., *Proc. SPIE* **7636**, 76361J (2010); Naulleau et al., *Proc. SPIE* **7985**, 798509 (2011)].

Structure-based drug design is focused primarily through the Berkeley Center for Structural Biology (BCSB) PRT on beamlines established for protein crystallography experiments. Protein crystallography is now a standard tool in the drug discovery process and often requires the intense x-rays available from light sources. It enables researchers to study the three-dimensional structure of target proteins at the atomic scale, to design molecules that are predicted to bind and inhibit their targets, and to test the target–inhibitor complex. The utility of the technique is highlighted by the results of companies such as CoCrystal Discovery, which uses structure-based design to develop anti-viral drugs, and Genentech, which has used structure-guided design to develop anti-cancer drugs such as trastuzumab, erlotinib, and bevacizumab. The technique is also used to optimize previously discovered drugs, as in the case of imatinib, a leukemia drug which was developed by Novartis through chemical library screening. Later, synchrotron x-ray data obtained on imatinib bound to its target showed that the drug was specific to a particular oncoprotein, which then paved the way for development of even more specific anti-leukemia drugs.

Another example is a small drug discovery company, located less than five miles from the ALS, called Plexxikon. Founded in 2003, the company has



Before and after scans of a patient treated with Zelboraf, an anti-melanoma drug developed with support from ALS research. Courtesy of the Peter MacCallum Cancer Centre.

continued on page 13

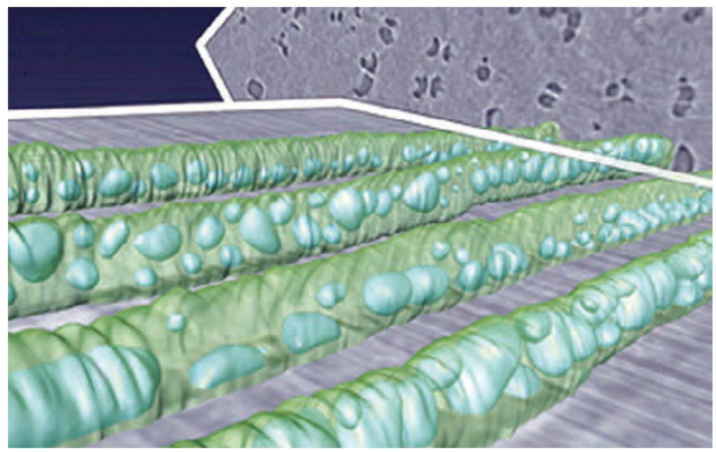
Industry Stories

continued from page 12

used ALS Beamline 8.3.1 to support the development of the anti-melanoma drug vemurafenib (trade name Zelboraf), which obtained Food and Drug Administration approval for use in 2011. The drug targets a mutated, active form of the B-Raf protein, which is present in about half of all cases of melanoma and promotes growth and division of the melanoma cells. The drug was so successful in human testing that trials were halted so that all patients in the trial could be treated. Zelboraf marked a significant advancement for patients with metastatic melanoma who historically have had very limited treatment options [Bollag et al., *Nature* **467**, 596 (2010)].

The ALS has numerous tools open to other industries studying specialized problems that require an intense x-ray source. When we include academic groups funded by industry, we find a diversity of industries that benefit from the ALS, including research in new materials, combustion, energy storage and conversion, and fundamental knowledge. For example, the Mitsubishi Rayon Corporation is exploring the production of high-quality carbon fiber. The Wood-Based Composites Center, a National Science Foundation Industry/University consortium, is using the ALS to investigate the performance of composite materials based on resin distribution. Improving batteries and moving beyond the lithium-ion battery is the focus of academic groups and members of the automobile industry working to improve electric cars. The wine and floral industries fund work to image the transpiration process in plants to understand their reaction to water stress.

Currently, user-facility access mechanisms for industrial users are undergoing nationwide review. A recent report from the Department of Energy's Basic Energy Sciences Advisory Committee (BESAC) highlighted the many challenges facing industry users wanting access to user facilities. The ALS recognizes that the slow, rigorous, peer-reviewed proposal process that grants access to academic groups can be a roadblock for industrial users, inconsistent with the need for rapid idea-to-solution turnaround times. Other modes of access do exist, and industry groups are invited to contact Sue Bailey (SBailey2@lbl.gov) to discuss their needs.



Visualizing drought recovery in plants. In vivo high-resolution x-ray computed tomography sections of a representative grapevine stem undergoing vessel refilling. The vessels that transport water through plants are vulnerable to blockage by gas bubbles that form during periods of drought.

Omar Yaghi

continued from page 1

show great promise as a method for carbon capture and potential carbon dioxide conversion to fuels. With the highest surface area and lowest densities in solids known to date, MOFs are a key component in the field of clean energy technology. And the building-block approach that Yaghi developed has launched a whole new field of research identified as "reticular chemistry." Yaghi and his research team continue their reticular chemistry research in the Materials Sciences Division at Berkeley Lab and through his concurrent position with the University of California, Berkeley's chemistry department.

Born in Amman, Jordan, Yaghi came to America as a teenager to pursue his education. He received his B.S. in chemistry from the State University of New York at Albany in 1985 and his Ph.D. from the University of Illinois at Urbana in 1990. He spent time as a postdoc at Harvard, then joined the faculty at Arizona State University. Yaghi became a professor of chemistry at the University of Michigan and then joined the UCLA faculty in 2005, where he became the director of the Center for Reticular Chemistry at the California NanoSystems Institute.

What initially attracted Yaghi to the field of chemistry—his fascination with the "hidden world" of molecular structures—still holds its appeal today. But the initial draw of science as a solitary career has changed as he's experienced the potential of scientific collaboration. It is this appreciation for what he terms "team science" that attracted him to Laurence Berkeley National Laboratory (LBNL) and the Foundry.

"A lot of inventions start with a researcher working in their own area, but to solve a big problem you need a team of scientists from a variety of disciplines to come together," says Yaghi. "I think that LBNL, and specifically the Foundry, does this very well."

Yaghi describes his impression after his first visit to the Foundry as sheer amazement with how the facility works. He sees the Foundry as a model for the rest of the world.

"We have scientists doing polymer chemistry, inorganic nanostructures, nano-imaging, theory, bioinspired materials, and nanofabrication, including

continued on page 14

THE ALS COMMUNITY

ALS ON THE EVE OF TURNING 20

by Roger Falcone

Roger Falcone

Next year will mark the 20th anniversary of the start of user support at the ALS. As we all can appreciate, maturity brings reflection, challenges, and opportunities.

When the ALS was first being considered, the importance of soft x-rays for science was challenged. Now, we see that others have emulated us. The ALS continues to be a leader in soft x-ray brightness and other technical capabilities, as well as in science that utilizes imaging, spectroscopy, scattering, and dynamics. However, we have seen enormous growth in soft x-ray science over 20 years, including the construction of other facilities worldwide. Competition and collaboration with those facilities has helped us to remain at the forefront in meeting the needs of science.

Our experience also means that we have learned to do many things exceptionally well: our skilled technical, administrative, and scientific staff smoothly assist users; we operate safely and very productively; and we have established a warm and supportive culture in the ALS Division. Reaching maturity means replacing and

upgrading older parts and planning carefully for the future. We are grateful for continued DOE support for our upgrades and renewal plans. This support has allowed us to engage new users as well as ones we have served for many years, all of whom offer helpful advice on future priorities for the facility.

On a global scale, all synchrotron facilities are spending time on introspection. One question is, "How can we justify the considerable and increasing resources we request

> "On a global scale, all synchrotron facilities are spending time on introspection."

from taxpayers?" I answer that we are getting better at serving societal needs by doing the basic science that leads to

continued on page 22

Omar Yaghi

continued from page 13

instrument-extensive work and synthesis-extensive work all in one spot and they are cooperating together across biology, chemistry, physics, and engineering," says Yaghi. "This is really quite powerful and I believe it is the way to address scientific challenges nowadays."

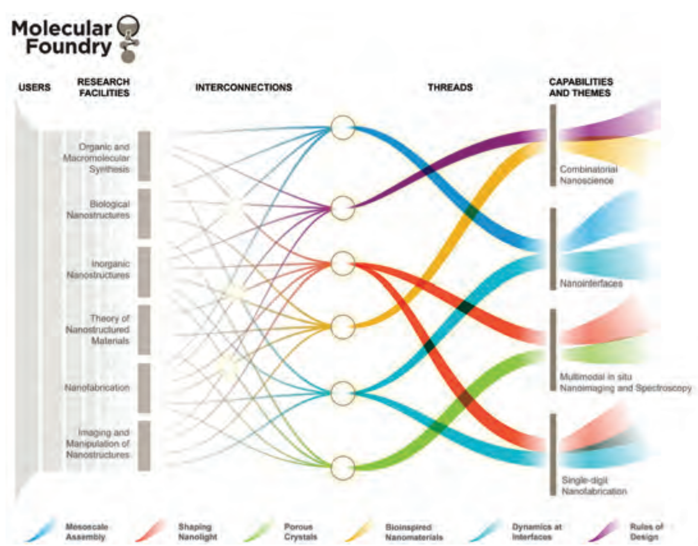
Much like the ALS, the Molecular Foundry hosts hundreds of users from all over the world each year who come to the facility to conduct their own research and tap into the depth of expertise of the staff scientists.

"Our scientists have a dual role of developing their own research but also teaching scientists from other institutions how to carry out particular scientific projects," says Yaghi. "Clearly, through these collaborations the Foundry is growing in its expertise and it's growing in what it offers its users."

Yaghi sees synergistic opportunities for collaboration with the ALS as well, both for Foundry users and staff scientists, and he's working with the ALS to develop deeper connections.

"I am very excited about the potential for collaboration between the ALS and the Foundry," says Yaghi. "For example, the

continued on page 23



Graphical representation of intertwining threads connecting users and research facilities with broader capabilities and themes at the Molecular Foundry.

STEVE KEVAN, NEW DEPUTY DIVISION DIRECTOR FOR SCIENCE

Steve Kevan

Steve Kevan has joined the ALS management team as Deputy Division Director for Science, effective July 2, 2012. Dr. Kevan, formerly Professor of Physics at the University of Oregon, is a longtime active ALS user and has been a member of the ALS Scientific Advisory Council for several years as well as a member, and chair, of the ALS Users' Executive Committee.

Dr. Kevan earned his Bachelor of Arts at Wesleyan University in 1976 and his PhD in Physical Chemistry from the University of California, Berkeley, in 1980, where he worked with former Berkeley Lab Director David Shirley. In his thesis work he pioneered the photoelectron diffraction technique for determining adsorbate surface structures and applied this to study sulfur, selenium, and CO adsorbed on low-index single-crystal nickel surfaces. After completing his PhD, Kevan worked at AT&T Bell Laboratories, where he developed new instrumentation for performing high-resolution angle-resolved photoemission at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. He focused in particular on high-resolution studies of intrinsic surface states on metal and semiconductor surfaces, discovering and characterizing many new states. In his final years at Bell Labs, Kevan applied an old idea called "dispersion compensation" to a new high-resolution electron scattering spectrometer.

At the University of Oregon since 1986, Kevan was an early participant in the planning stages of the ALS. He moved his research program, which focused on surface electronic structure and surface Fermiology, from the NSLS to the ALS to take advantage of the constantly improving resolution and capabilities at the facility. In the past decade, Kevan's research activities have increasingly focused on utilizing the high optical brightness of undulator radiation. He and his collaborators have used the high coherent flux available to pioneer the soft x-ray analogs of speckle metrology and dynamic light scattering. He led the construction of Beamline 12.0.2.2, which was an early step toward a dedicated and flexible coherent soft x-ray scattering and imaging beamline that is culminating with the construction of the COSMIC facility.

CORIE RALSTON: NEW HEAD OF BCSB

Corie Ralston's appointment as Head of the Berkeley Center for Structural Biology (BCSB) has her busy looking at budgets, funding, and big-picture goals. The biophysicist staff scientist has been with BCSB for more than 10 years, so much of what she's considering comes from an intimate familiarity with the day-to-day operations and challenges of the facility.

In her beamline research, Ralston studies chaperonin protein structures, which she describes as "the really important medics in our cells" that can fix misfolded proteins. Since misfolded proteins may cause many diseases, such as Alzheimer's and Parkinson's, a better understanding of chaperonins could lead to breakthrough drug developments. Ralston's research is part of a collaboration with Stanford that was organized by former BCSB Head Paul Adams.

Beamline engineering developments are what keep Ralston's crystallography work moving forward, and managing this process will be key to her new position as Head of BCSB. From software tools that advance data processing and collection to hardware tools like beamline optics and robotic controls, engineering development is what keeps the ALS crystallography beamlines at the forefront. "It's a challenge because whenever you're doing something new that increases the flux of the beamline, you're in danger of making it less stable," says Ralston. "Maintaining this balance between stability and technological advancement is one of our biggest challenges."

Besides maintaining existing BCSB funding—the majority of which comes from contracts with participating research teams (PRTs), Howard Hughes Medical Institute, and an NIH grant—Ralston hopes to develop new funding sources by restructuring beamline contracts. She'd like to be able to offer smaller amounts of guaranteed beamtime to PRT users with smaller budgets, which is a more common situation in today's economy. Ralston would then launch an aggressive public relations campaign, travelling to present the new option to companies and academic institutions nationwide. "I would really love BCSB to be the first thing someone thinks of when they need to solve a structure in order to move forward with their research," says Ralston.

Corie Ralston

THE ALS COMMUNITY

USERS' EXECUTIVE COMMITTEE UPDATE

by Brandy M. Toner, 2012 UEC Chair

As the 2012 chair of the Users' Executive Committee (UEC), I serve the users of the ALS along with 11 elected members. The goal of the UEC is to represent the interests of users to the Department of Energy and ALS management. The UEC Charter can be viewed at the ALS Web site by following the User Information/User's Executive Committee link from *http://www-als.lbl.gov/*. The UEC meets quarterly with ALS management and staff to discuss issues affecting users. Whenever user issues arise, please feel free to contact individual UEC members or the entire committee at alsuec@lbl.gov. You can join the UEC by running for election in the fall of 2012: become a UEC candidate by contacting nominating committee co-chairs David Kilcoyne (ALKilcoyne@lbl.gov) and Jeffrey Kortright (JBKortright@lbl.gov).

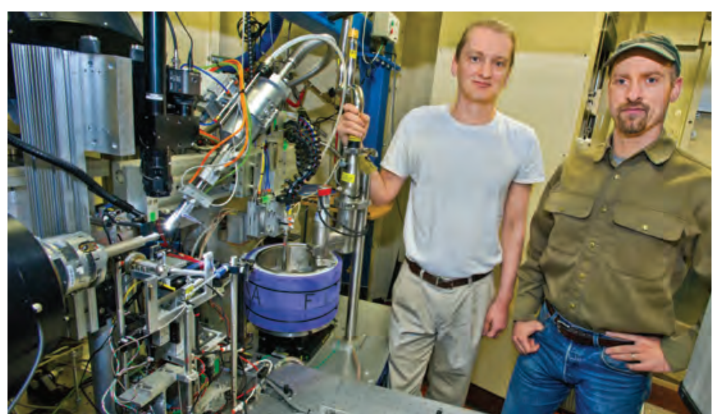
The ALS and UEC members are also active on behalf of users at the national level through elected positions in the National User Facility Organization (NUFO). The goal of NUFO is to represent the interests of users of national facilities in the United States. ALS UEC member Yves Idzerda (Montana State University) was recently elected vice-chair of the NUFO Steering Comittee, and ALS User Services Group Leader, Sue Bailey, was elected vice-coordinator. The annual NUFO meeting will be hosted by the ALS in 2013. Please contact the UEC or ALS User Office about how you can get involved in the next NUFO annual meeting.

The ALS User Meeting is a major activity of the UEC. This year, program co-chairs, Peter Nico (Berkeley Lab) and Chris Cappa (University of California, Davis), 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 8–10, 2012, to celebrate the scientific accomplishments of the past year and learn what is next in synchrotron research at the meeting workshops.

UEC members who attended the February 2012 meeting, from left: Jan Liu (student member), Jeff Kortright, Yuri Suzuki, David Osborn, Brandy Toner, David Kilcoyne, Hendrik Bluhm, Chris Cappa, and Peter Nico.

R&D 100 AWARD FOR THE DEVELOPMENT OF THE COMPACT VARIABLE COLLIMATOR

A team led by **Simon Morton** and **Jeff Dickert** of Berkeley Lab's Physical Biosciences Division has been awarded an R&D 100 Award for the development of the Compact Variable Collimator (CVC). The CVC, installed at the ALS Berkeley Center for Structural Biology (BCSB) beamlines, is small, easy to use, and readily adapted to any configuration of an x-ray beamline, where it allows researchers to quickly and accurately adjust x-ray beams for protein crystallography, x-ray microscopy, and small-angle x-ray scattering to optimize resolution. This optimized resolution allows researchers to extract the highest-quality data from less-than-perfect protein crystals rather than discard crystals with defects and spend time and money preparing new ones. The CVC has already been used to make critical discoveries in areas that include Alzheimer's and Parkinson's disease, Lassa fever, antibiotic resistance, and food crop improvements. Co-nominating the CVC with Berkeley Lab were Takeda Pharmaceutical and the Genomics Institute of the Novartis Research Foundation.



Simon Morton and Jeff Dickert in hutches at Beamline 5.

THE ALS COMMUNITY

EARLY CAREER RESEARCH AWARDS

Feng Wang

Kevin Wilson

Oliver Gessner

Three ALS users have been recognized with prestigious Early Career Research Awards, one from the White House and two from the DOE.

Feng Wang of Berkeley Lab's Materials Sciences Division was one of 94 recipients in 2011 of the Presidential Early Career Awards for Scientists and Engineers, the highest honor bestowed by the United States government on science and engineering professionals in the early stages of their independent research careers. Wang was cited for "pioneering research on ultrafast optical characterization of carbon nanostructures that has advanced the fundamental understanding of the electronic structure of graphene and is expected to enable the development of advanced-energy-relevant technologies." Wang was previously an ALS doctoral fellow on Beamline 8.0 and is an ALS user on Beamline 1.4. "For a young scientist the first years are the most critical," says Wang, who focuses on the fundamental science and potential applications of graphene's optoelectronic properties. "The Presidential Early Career Award provides not only financial support but encouragement, letting us know that we're doing well. I am extremely happy and honored by this award. It will have a huge impact on my work."

Kevin Wilson, a beamline scientist on the Chemical Dynamics Beamline 9.0.2, has been granted an Early Career Research Award by the DOE's Office of Science. The five-year awards are designed to bolster the nation's scientific workforce by providing support to exceptional researchers during the crucial early career years, when many scientists do their most formative work. The research awards also aim at providing incentives for scientists to focus on mission research areas that are a high priority for the DOE and the nation. Wilson's work focuses on hydrocarbon free radicals formed at hydrocarbon/water and electrolyte interfaces. He plans to use his research award to study the roles they play in chemistry as initiators or propagators of surface reactions or as reactive intermediates.

Berkeley Lab scientist and ALS user **Oliver Gessner** is another recipient of the DOE Early Career Research award. Gessner, who is associated with Berkeley Lab's Chemical Sciences Division, will use his award to study the role that chemically engineered devices play in the development of sustainable energy production and storage solutions. He'll employ experimental techniques using intense, ultrashort x-ray pulses to monitor the light-induced creation and transport of charges in complex molecular systems in real time and from the perspective of specific atomic sites.

SSG: Maestro *continued from page 7*

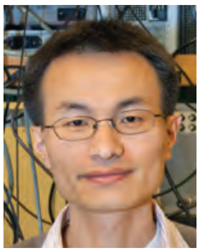
both fundamental and practical material sciences."

New Science. The following selected highlights from the past year not only reflect world-class science but also illustrate the unique capabilities made available at the ALS by the SSG.

- Hidden Rotational Symmetries in Magnetic Domain Patterns, *Phys. Rev. Lett.* **107**, 257204 (2011). http://www-als.lbl.gov/index.php/science-highlights/science-highlights/676
- Lensless Imaging of Magnetic Nanostructures, *Phys. Rev. Lett.* **107**, 033904 (2011). http://www-als.lbl.gov/index.php/science-highlights/science-highlights/648
- Two Phase Transitions Make a High-Temperature Superconductor, *Science* **331**, 1579 (2011). http://www-als.lbl.gov/index.php/science-highlights/science-highlights/599
- Lensless X-Ray Imaging in Reflection, *Nat. Photonics* **5**, 243 (2011). http://www-als.lbl.gov/index.php/science-highlights/science-highlights/595
- Large Magnetization at Carbon Surfaces, *New J. Phys.* **12**, 123012 (2011). http://www-als.lbl.gov/index.php/science-highlights/science-highlights/580

THE ALS COMMUNITY

HONORS AND AWARDS



Peidong Yang, an ALS user from Berkeley Lab's Materials Sciences Division and a Professor of Chemistry at UC Berkeley, was elected to the 2012 class of the American Academy of Arts and Sciences. Yang, a chemist whose research focuses on the synthesis of new classes of materials and nanostructures, is expert on nanowires and has found ways to use them for photovoltaics and as a thermoelectric material. Earlier this year, Yang was named by Thomson Reuters as the world's top materials scientist of the past decade and the tenth most influential chemist, based on an analysis of the citation impact of published papers.

Brandy Toner, an ALS user from the University of Minnesota and UEC chair, has been named the National Science Foundation Ridge 2000 Distinguished Lecturer for 2011. Toner, an assistant professor at the University of Minnesota, studies the biogeochemical processes that move metals through pristine and contaminated environments. She is particularly interested in the mineralogy and chemistry of hydrothermal plumes. A specialist in synchrotron radiation spectroscopy and diffraction technologies, Toner is using novel tools to address these questions, leading to exciting discoveries at hydrothermal vent sites around the globe.

James Berger, an ALS user from the Physical Biosciences Division, was also elected to the 2012 class of the American Academy of Arts and Sciences. Berger is a biochemist and structural biologist who studies protein machines and develops models to explain DNA replication, chromosome superstructure, and other essential nucleic acid transactions. Last year he received the National Academy of Sciences Award in Molecular Biology "for elucidating the structures of topoisomerases and helicases and providing insights into the biochemical mechanisms that mediate the replication and transcription of DNA."

Jim Floyd, the ALS Environment, Health, and Safety Program Manager, was a recipient of the Berkeley Lab Director's Award for Exceptional Achievement in Safety. Floyd's award, announced in May 2012, was in recognition of his "Accomplishments and leadership in promoting a safety culture."

OUTREACH TO THE SCIENTIFIC AND LOCAL COMMUNITIES

by Elizabeth Moxon

The ALS Communications Group is always looking for new ways to promote ALS science and engineering to other scientists, potential users, stakeholders, and the general public. From our ongoing bimonthly Science Cafés and participation in the annual Open House, to our active roles in national and international scientific and communications organizations, our goal is to keep all our audiences informed about ALS capabilities, the exciting science, and the great people who work here.

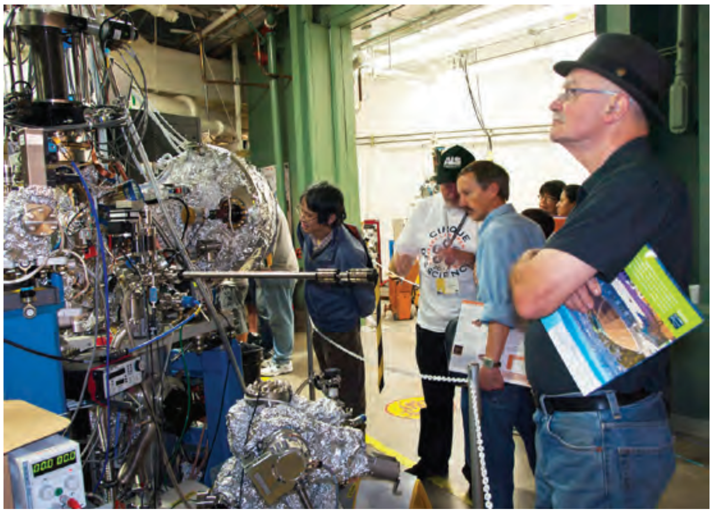
ALS staff, beamline scientists, and users all pitched in to make the 2011 Open House event, held last October, another huge success. From 10:00 a.m. to 3:00 p.m., more than 1300 eager visitors from the community came to see what happens "under the dome." Before beginning a self-guided tour around the ring, all were greeted by Division Director Roger Falcone and Deputy for

Posing at the ALS souvenir "Photo Booth."

continued on page 19

THE ALS COMMUNITY

Outreach *continued from page 18*



Visitors to the experiment floor during the 2011 Open House were fascinated by the equipment, the science, and yes, the foil.

Operations, Banda, who gave brief overviews of the history of the ALS, how it works, and what kinds of scientific research are enabled by brilliant x-rays. Around the ring, more than 60 hardy volunteers were stationed by beamlines, video demonstrations, survey and alignment equipment, and science posters, ready to answer the visitors' questions. A particular highlight was the "ALS Photo Booth" where people could stand by a beamline and have their photo taken by a staff member who also belongs to the LBNL Photography Club. The result is a charming YouTube video *(http://tinyurl.com/als-visitors)* featuring smiling families, friends, Boy Scouts, students, staff, and more. Upon leaving the ALS, many visitors stopped to give their impressions of the facility and of the staff they met as they walked around the experiment floor; see their comments—including the Boy Scouts'—at *http://tinyurl.com/open-house-impressions.* This year's Open House will be held on Saturday, October 13.

Users and staff continue to fill the room for the bi-monthly ALS Science Café. Organized by ALS Communications and hosted by Roger Falcone, the cafes feature three scientists providing brief overviews of their work, followed by engaging—and often spirited—discussions. The lunchtime events have become an excellent venue for scientists and nonscientists to hear about the breadth of ALS science, while also promoting opportunities for collaboration. Recent topics have included the study of extraterrestrial materials, self-assembly of proton-conducting block copolymers, materials with memory, molecular mechanisms of proteins, and more. The entire list of speakers and topics can be viewed on the ALS Web site at *http://tinyurl.com/als-sci-cafe.*

Reaching beyond the local community, group members have become involved in a variety of communications and science organizations, focusing on engaging the public, media, stakeholders, scientists, and users by publicizing the work done at light source facilities around the country and the world. The National User Facility Organization (NUFO) meets annually to assess the needs of users who conduct research at U.S. national research facilities. This year, ALS UEC member Yves Idzerda was elected to the position of vice-chair, and he will assume the leadership next year. User Services Group Leader Sue Bailey is vice-coordinator, and the communications staff joined a new NUFO committee that will explore using novel multimedia strategies to engage new audiences. The NUFO collaboration also serves to inform the public and stakeholders about the contributions of national user facilities by creating workshop reports on industry usage and educational outreach and by organizing a poster session on Capitol Hill each year to showcase research to members of Congress. Further outreach to Congress from the ALS took the form of a new handout, known informally as the "ALS Sampler." Designed to provide an easily accessible snapshot of current research and facility information to busy executives and public officials, the handout was passed out to congressional staff this winter.

Filling out questionnaires at the lightsources.org facilities poster exhibit at SRI 2012.

ALS Science Café.

At the international level, ALS outreach includes attending scientific conferences and providing brochures, handouts, and staff to inform the international scientific community about the possibilities of conducting research on ALS beamlines. In addition to representing the ALS at conferences, we also serve on the management board and support lightsources.org, the international collaboration of synchrotron communicators. Most recently, lightsources.org funded a facility poster display at SRI 2012, held in Lyon, France. The exhibit featured 35 facility posters from light sources around the world and attracted a constant stream of conference attendees. The many visitors to the exhibit were asked to fill out a questionnaire about what kind of information they would like to see on the lightsources.org Web site, which is currently undergoing a complete redesign to better serve users and staff; their input has already contributed to what will appear on the new homepage.

Scientific and educational outreach will continue to be a primary focus of the ALS Communications Group. ALS users and staff are always invited to send us new ideas on how to reach and expand our audiences, by emailing us (alscommunications@lbl.gov) or by visiting in person on the third floor of the User Support Building (Bldg 15).

FACILITY UPDATES

ACCELERATOR AVAILABILITY AND RELIABILITY

by Christoph Steier, David Robin, and David Richardson

Similar to other light sources, the ALS operating schedule is divided into user beam, accelerator physics/startup/machine setup, maintenance and installation, and vacation/holiday shifts. In a "typical year," there is usually one long shutdown for major maintenance, large installations, and upgrades to the accelerator as well as user beamlines. The length of the shutdown period is not fixed and depends on the scope of the work. With many upgrades going on as part of the ALS strategic plan, recent shutdowns have been longer and larger in scope than during earlier years of operations. Usually, the ALS schedules and delivers more than 5000 beam hours to users per year.

Availability is one of the most important performance parameters of the facility. Availability is defined as the ratio of delivered versus scheduled user time. The DOE goal for availability is >90%, whereas the ALS internal goal is >95%. Maintaining a high availability as the facility becomes more mature and complex has been a challenging task. The table shows the availability of the ALS for the last three fiscal years.

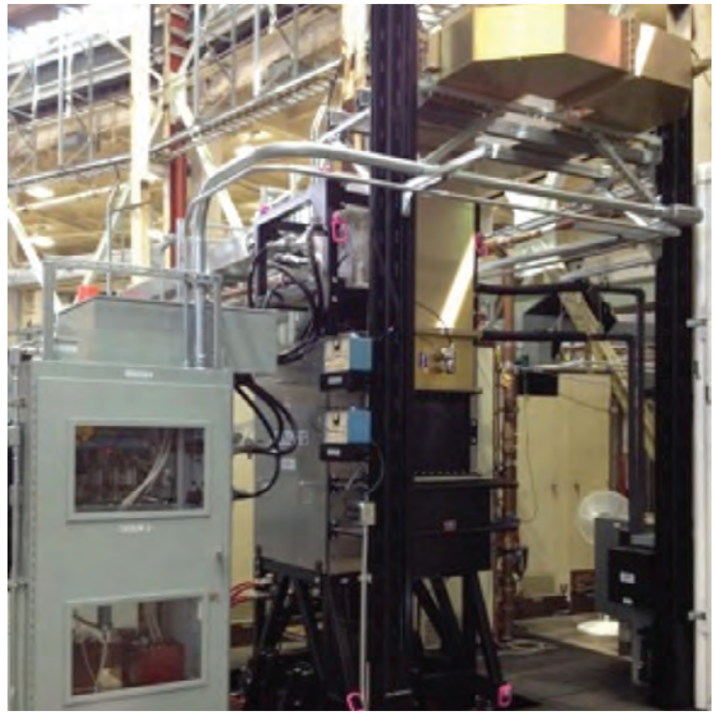
Over the last years, the distribution of shutdowns has been somewhat irregular, based on the timing of major pieces of equipment (rf, power supplies) being ready for installation. There were nearly 6000 user hours scheduled in FY10, with the ALS running the entire year without a major shutdown. This resulted in two major shutdowns falling into FY11, resulting in just below 5000 scheduled user hours. Since February 11, 2009, the ALS has been run almost exclusively in top-off mode. During this period, the availability has been better than in the preceding years. Also, an additional 136 hours (2.3%) of unscheduled light were delivered to users in FY10, and an additional 80 hours (1.6%) were delivered in FY11.

Reliability is another important performance parameter of the facility, which is distinct from availability. 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 table also shows the MTBF numbers for the last three fiscal years. In FY11 we achieved an MTBF of almost 47 hours, just shy of our goal, which remains to increase the MTBF to be reliably above 48 hours (less than 1 fault per two days).

Hours Scheduled and Delivered

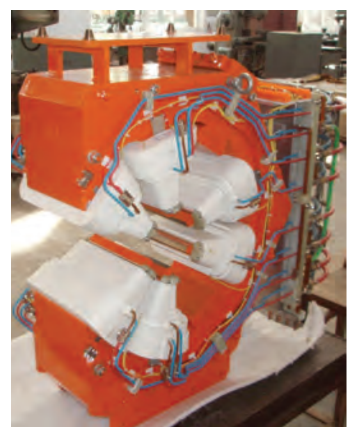
	Scheduled hours	Delivered hours*	Availability	Mean time between failures (hours)
FY09	5471	5278	96.5%	37.4
FY10	5980	5707	95.4%	32.4
FY11	4939	4836	97.9%	46.6

*Does not include unscheduled hours delivered to users.



New rf klystron operational since January 2012.

There are ongoing programs to analyze every single fault, analyze fault patterns, and develop improvement programs. As part of this, many major systems were identified over the years and the ones that have been responsible for larger numbers of faults are being actively addressed. This includes faults coming from water clotting, power-supply failure, external power glitches, aging core controls, and the rf power system. The improvements span from improved monitoring and intensified preventive maintenance to full system replacement. Many of the smaller improvements have already resulted in better availability and MTBF in FY11. The major shutdowns during the last year saw significant new hardware being installed, including a new rf klystron, several new major power supplies, new low-conductivity water pumps, and parts of the replacement control system. Immediately after those shutdowns, there were small "teething" effects due to the new equipment, but after resolving those issues, the new systems have been reliable. Overall,



One of 48 new sextupole magnets to be installed next year as part of the brightness upgrade.

continued on page 21

FACILITY UPDATES — USER DEMOGRAPHICS AND PUBLICATIONS

by Sue Bailey

As a national user facility, the ALS is required to report comprehensive user demographics and publication information annually to the U.S. Department of Energy. A sampling of that information is reproduced here. Figure 1 shows the overall user numbers in various scientific fields over time (FY07–FY11). Beginning in 2010, we began counting the growing numbers of remote users, primarily from the life sciences. These users save time, energy, and money by shipping their samples to the ALS and remotely operating the beamline to collect their data. Figure 2 shows the different categories of researchers at the ALS. Over half our researchers are young trainee scientists who will make key contributions to U.S. competitiveness in the future. Figure 3 shows the scientific productivity of the ALS as measured in refereed and high-impact journal articles since 1994. The designation "high-impact" includes journals with an impact factor greater than 7.2.

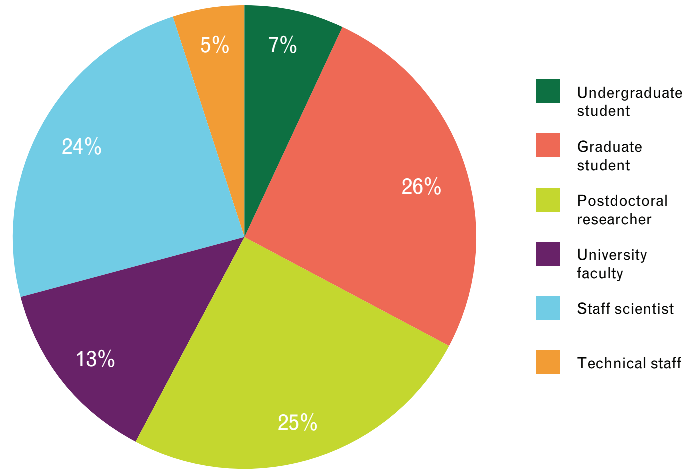


Figure 2. Pie chart showing the different categories of researchers at the ALS.

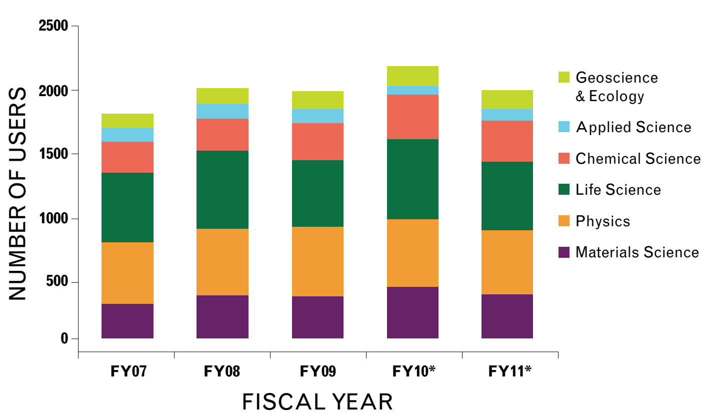


Figure 1. Bar graph showing the relative numbers of users in various areas of science. *FY10 and FY11 include remote users.

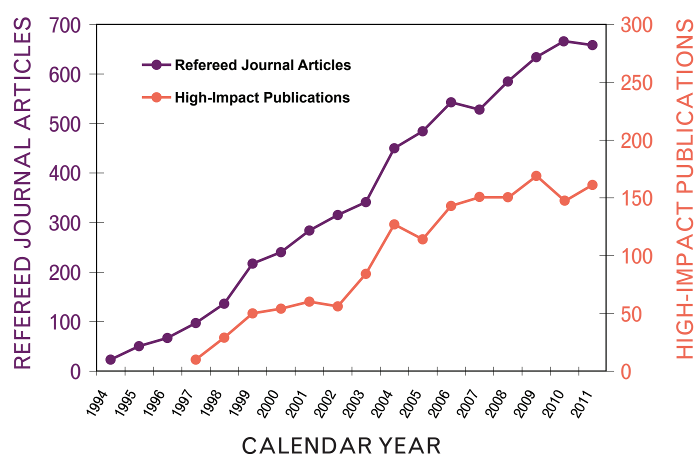


Figure 3. Graph of growth in refereed journal articles and high-impact publications.

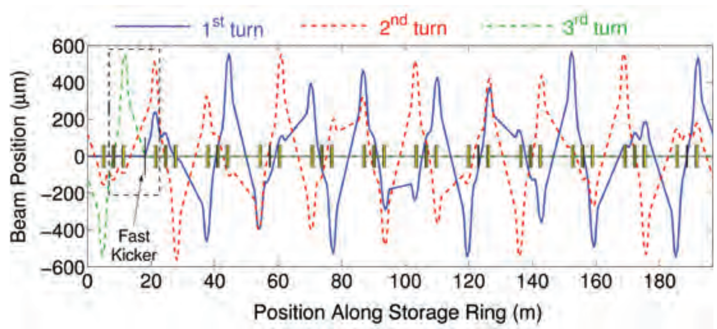
Beam Delivery *continued from page 20*

through July 2012, the availability for FY12 is 96.0% and the MTBF is 38 hours, a good performance considering the scope of the ongoing upgrades.

In parallel with the current upgrades, which are mostly aimed at improving reliability as well as energy efficiency, much work is also going on for the next stages of accelerator upgrades. Production of the new sextupole magnets for the brightness upgrade is complete. This will enable a significant improvement in brightness next year. New beam-position monitors are being developed under the leadership of NSLS-2 in collaboration with ALS and SPEAR and have been tested at the ALS. This will enable an improvement to the orbit feedbacks and orbit stability. There also are plans to improve beam-size stability as part of the brightness upgrade, by adding 24 additional skew quadrupoles. Finally, new insertion devices (elliptically polarizing undulators) with tailored period lengths are being built for several new (and one existing) beamlines as part of the ALS strategic plan.

Falcone *continued from page 14*

U.S. Congressman John Garamendi (center) and a meeting of his Manufacturing Advisory Committee (MAC) were hosted at the ALS User Support Building last November. The MAC is made up of business and labor leaders from throughout California's 10th Congressional District and the East Bay.



A recent experiment in pseudo single-bunch mode demonstrated the feasibility of a "kick-and-cancel" scheme where, after two full turns around the storage ring, the orbit of the kicked bunch returns to its zero position in such a way that a second kick cancels the perturbation. The kick-and-cancel process can be repeated "on demand," thus creating single-bunch pulses with adjustable pulse repetition rates.

improved technologies, in addition to our traditional role of fundamental discovery. ALS research that supports technology is leading to better health through an understanding of biological structure and function, faster computers through advanced short-wavelength lithography, and sustainable energy technologies with in situ measurements of operating devices.

Another introspective question is, "What will be the role of storage-ring x-ray sources when linear x-ray free-electron lasers (FELs) become more common?" I answer that we should upgrade our storage ring to produce even brighter and more stable coherent light, for applications including spectroscopy and imaging, while we also see a wonderful future for the fast and powerful x-ray pulses from new FELs, enabling ultrafast dynamics. At the ALS, we are thinking long-term about replacement of all of the core parts of our storage ring, in addition to near-term upgrades of insertion devices, optics, and detectors on all our beamlines. We are engaged in international discussions around such "ultimate storage rings." The footprint of the ALS allows for consideration of such a future upgrade in addition to the Next Generation Light Source (NGLS) FEL currently under consideration at the Lab.

There are also questions about fiscal challenges for the DOE and Congress in supporting an increasing number of scientific facilities, nationally. However, our political representatives and industrial leaders, who are visiting us more and more often these days, have been pleased to observe that we serve a broad spectrum of scientists who benefit in diverse areas of research from the impressive and broad set of tools we provide. Important synergies exist between the capabilities we have to use x-rays to look inside functioning systems, and new scientific programs of individual principal investigators in universities, labs, and industry. Examples of new programs (supporting new communities of ALS users) include a center for artificial photosynthesis (looking for a way to efficiently convert sunlight to fuel), a proposed center in energy storage (looking to improve batteries), and a proposed center in energy-critical materials (looking for alternatives to the expensive and rare materials that go into technologies such as cell phones, wind power, and cars).

While these introspective questions form the backdrop for our 20-year anniversary, and I hope I have conveyed my sense that the answers form great opportunities, we also have day-to-day challenges, which I believe we are making great progress in meeting.

For example, while we have an excellent safety record, our work planning continually needs to be refined. A recent electrical shock incident, even though proper GFCI protection was in place limiting it to non-

Safety is Elemental

hazardous energy, reminds us that we cannot get complacent.

Around the ring we can see a lot of changes. We have constructed and recently inserted our newest undulator in Sector 6. Planning continues on the new COSMIC and MAESTRO Beamlines in Sector 7, where the construction phase will start with the removal of the current beamlines toward the end of this year. We are working with DOE to find funds for our proposed AMBER beamline for Sector 8.

Our sextupole magnets are beginning to arrive, and we will install them in the storage

continued on page 23

Falcone continued from page 22

Roger and Joy Kono pose for a photo at her retirement party in June.

ring during the extended shutdown in January 2013, when we will also install new components as part of our four-year control system upgrade. In a recent test of what we call "pseudo single-bunch mode," our Accelerator Physics Group demonstrated a unique new capability where we kick a single electron bunch into a new orbit in the storage ring, resulting in isolated and intense x-ray pulses at controllable repetition rates (up to MHz) that can be synchronized with controlled perturbations on samples, for measurements of dynamics at multiple beamlines.

As we reach the final phase of several projects funded under the American Reinvestment and Recovery Act (stimulus funds), we're looking forward to the installation of new high-speed-readout CCD detectors built at LBNL. These detectors are also sought by other facilities worldwide, but we look forward to employing them here first.

We have a number of new faces at the ALS. I will mention two folks who work with me daily: Yeen Mankin (from the Computational Research Division at the Lab) took over from Joy Kono, my wonderful and long-time assistant who retired this June; Steve Kevan (from the University of Oregon) became Deputy for Science. Steve knows the ALS well, as he has been involved on our advisory committees and as a user since the start of ALS. I thank Ben Feinberg for his great work as interim Science Deputy when Bob Schoenlein assumed leadership for science for the proposed NGLS project. Fortunately, Ben and Bob, together with Janos Kirz, continue to advise us. To return to my first topic, it's great to have such folks around, those who have a broad perspective, when you're turning 20 and embarking on serious introspection.

Yeen Mankin is now a part of the ALS team as Roger's assistant.

Omar Yaghi continued from page 14

ALS can really help us decipher what is happening between reactants and products in chemical and physical transformations."

Understanding how solid-state materials form is one of the first things that comes to mind when Yaghi ponders opportunities for ALS/Foundry collaboration. He describes the process of making solid-state materials as similar to a black box—you put something in and you get something out, but in the middle it is like a black box and so the process by which the material forms is largely an unknown. The ALS could help shed light on this process, says Yaghi.

Yaghi's vision of a scientist's job includes inspiring early career scientists, and he believes that a very good way to inspire them is to show them something that they thought could not be achieved. He sees a role for the ALS in this arena as well: shedding light on the sequencing of chemical groups within complex materials.

With his arrival at the Foundry coming about seven years after the first scientists began working at the facility, Yaghi says he sees that the Department of Energy (DOE) and LBNL vision for the Foundry is starting to bear fruit. He adds that this is really a statement on the quality of the work that Foundry scientists are doing and on the enlightened leadership of those who preceded him in guiding what he feels has become a precious national resource.

"Our scientists are progressively getting recognized for their unique contributions, being invited all over the world to give talks about their research and getting published in some very high-profile journals," says Yaghi.

"Our vision for the future is to identify what the world is going to be like in five or ten years and how we can prepare ourselves to meet the scientific challenges we'll be facing, says Yaghi. "The Foundry will be a great resource as we expand our efforts to include even more user researchers."

> "A lot of inventions start with a researcher working in their own area, but to solve a big problem you need a team of scientists from a variety of disciplines to come together. I think that LBNL, and specifically the Foundry, does this very well."

Science Roundup

continued from page 3

Dynein Motor Domain Shows Ring-Shaped Motor, Buttress

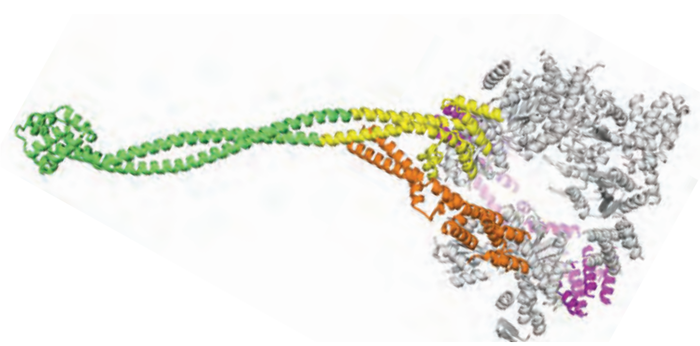
Carter et al., *Science* **331**, 6021 (2011)

Movement is fundamental to life. It takes place even at the cellular level where cargo is continually being transported by motor proteins. These tiny machines convert the energy gained from hydrolysing ATP into a series of small conformational changes that allow them to "walk" along microscopic tracks. Motor proteins (in the kinesin and myosin families) have been extensively studied by x-ray crystallography, but until recently there was little molecular structural information for dyneins. A group working at Beamline 8.3.1 has reported the 6-Å-resolution structure of the motor domain of dynein in yeast. It reveals details of the ring-shaped motor as well as a new, unanticipated feature called the buttress that may play an important role in dynein's mechanical cycle.

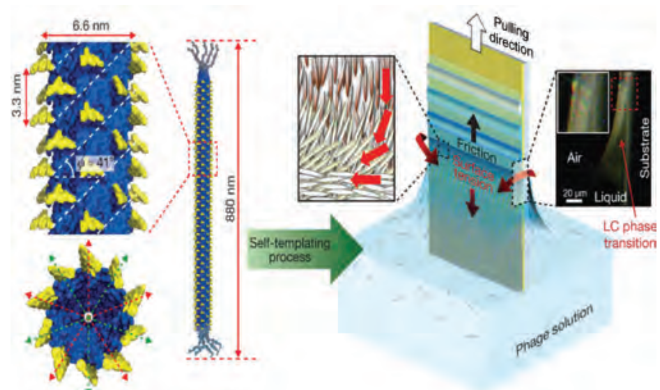
Highly Structured Biomimetic Materials

Chung et al., *Nature* **478**, 364 (2011)

Natural biological tissues are often hierarchically structured, and these structures appear to correlate strongly with tissue properties and functionalities. Finding out how a tissue self-assembles from cellular proteins has captured the interest of many biologists and material scientists who are interested in borrowing from nature's bag of tricks to synthesize artificial materials with desired properties. A team of scientists has recently discovered a method for controlling the assembly of such complex structures covering a large area from identical helical building blocks, in this case a rod-shaped virus, an accomplishment that could accelerate the development of diverse functional materials. Grazing-incidence small-angle x-ray scattering (GISAXS) measurements conducted on ALS Beamline 7.3.3 revealed the pseudo-hexagonal packed structure of the liquid-crystalline films.



Model for the whole dynein motor domain including the stalk (yellow) and its interaction with the buttress (orange).



Schematic diagram of the phage-based self-templating process. Left: The phage structure covered by about 2,700 alpha-helical major coat protein subunits. Right: The morphology is controlled by competing interfacial forces at the meniscus where liquid-crystal phase transitions occur. The polarized optical microscopy image shows iridescent colors originating from liquid-crystal phase formation at the air-liquid-solid interface.

BERKELEY LAB
Lawrence Berkeley National Laboratory

U.S. DEPARTMENT OF ENERGY
Office of Science

ALS ADVANCED LIGHT SOURCE

For information about using the ALS, contact:

ALS User Office
Advanced Light Source
Lawrence Berkeley National Laboratory
MS 6R2100
Berkeley, CA 94720-8226
Tel: (510) 486-7727
Fax: (510) 486-4773
Email: alsuser@lbl.gov

ALS home page
http://www-als.lbl.gov/

Editors:
Lori Tamura
Elizabeth Moxon
Shauna Kanel
Keri Troutman
Art Robinson

Design, layout, and photography provided by the Creative Services Office and the Communications Department of Berkeley Lab's Public Affairs Department.

The editors gratefully acknowledge ALS users and staff for their contributions, advice, and patience.

AUGUST 2012
Ernest Orlando Lawrence Berkeley National Laboratory
University of California
Berkeley, California 94720-8235

This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

The ALS is an Office of Science User Facility.

CSO24578