BNL-94685-2010

DISCOVERY *at Light Speed*

Photon Sciences Directorate at
Brookhaven National Laboratory

2010 ANNUAL REPORT

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The Photon Sciences Directorate at Brookhaven National Laboratory operates the National Synchrotron Light Source (NSLS) and is constructing the National Synchrotron Light Source II (NSLS-II). NSLS and NSLS-II are Office of Science User Facilities supported by the U.S. Department of Energy Office of Science.

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BROOKHAVEN NATIONAL LABORATORY

BNL-94685-2010
UC400
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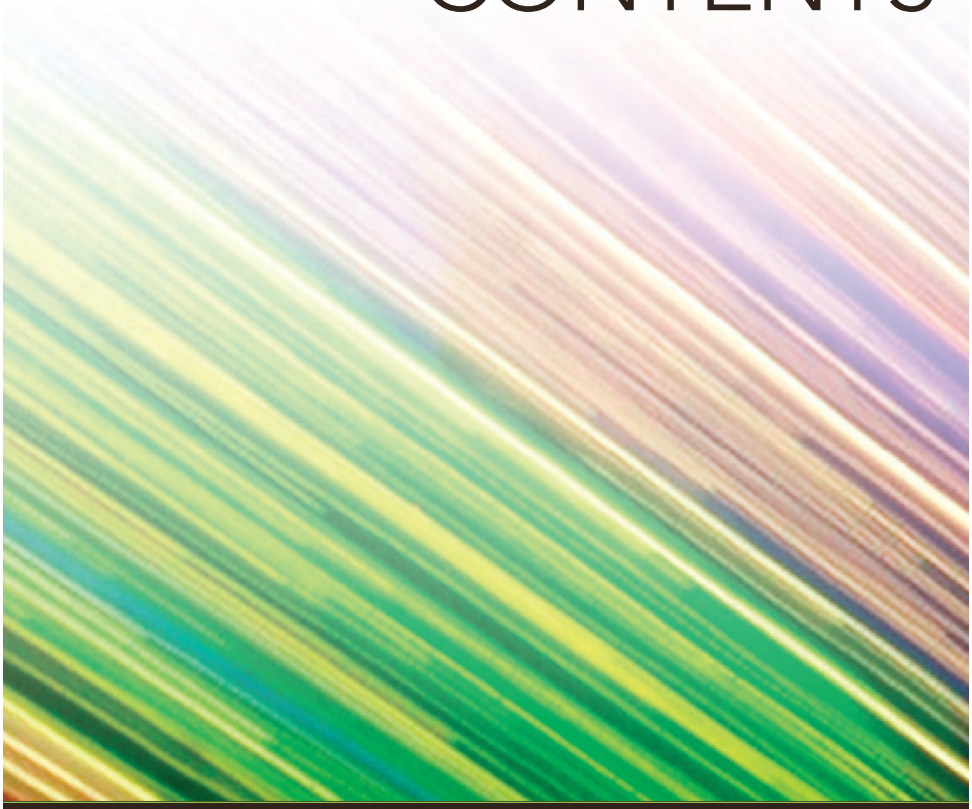

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REFLECTIONS ON THE YEAR

This is a very exciting period for photon sciences at Brookhaven National Laboratory. It is also a time of unprecedented growth for the Photon Sciences Directorate, which operates the National Synchrotron Light Source (NSLS) and is constructing NSLS-II, both funded by the Department of Energy's Office of Science.

Reflecting the quick pace of our activities, we chose the theme "Discovery at Light Speed" for the directorate's 2010 annual report, a fiscal year bookended by October 2009 and September 2010.

The year began with the news that NSLS users Venki Ramakrishnan of Cambridge University (also a former employee in Brookhaven's biology department) and Thomas A. Steitz of Yale University were sharing the 2009 Nobel Prize in Chemistry with Ada E. Yonath of the Weizmann Institute of Science.

Every research project has the potential for accolades. In 2010, NSLS users and staff published close to 900 papers, with about 170 appearing in premiere journals. Those are impressive stats for a facility nearly three decades old, testament to the highly dedicated team keeping NSLS at peak performance and the high quality of its user community.

Our NSLS users come from a worldwide community of scientists using photons, or light, to carry out research in energy and environmental sciences, physics, materials science, chemistry, biology and medicine. All are looking forward to the new capabilities enabled by NSLS-II, which will offer unprecedented resolution at the nanoscale. The new facility will produce x-rays more than 10,000 times brighter than the current NSLS and host a suite of sophisticated instruments for cutting-edge science.

Some of the scientific discoveries we anticipate at NSLS-II will lead to major advances in alternative energy technologies, such as hydrogen and solar. These discoveries could pave the way to:

- catalysts that split water with sunlight for hydrogen production
- materials that can reversibly store large quantities of electricity or hydrogen
- high-temperature superconducting materials that carry electricity with no loss for efficient power transmission lines
- materials for solid-state lighting with half of the present power consumption

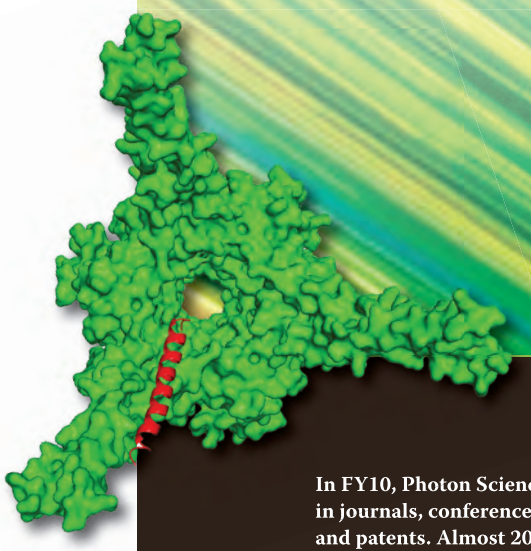
Excitement about NSLS-II is evident in many ways, most notably the extraordinary response we had to the 2010 call for beamline development proposals for the anticipated 60 or more beamlines that NSLS-II will ultimately host. A total of 54 proposals were submitted and, after extensive review, 34 were approved. Funding from both the Department of Energy and the National Institutes of Health has already been secured to support the design and construction of a number of these beamlines.

FY11 is a challenging and exciting year for the NSLS-II Project as we reach the peak of our construction activity. We remain on track to complete the project by March 2014, a full 15 months ahead of schedule and with even more capabilities than originally planned. The Photon Sciences Directorate is well on its way to fulfilling our vision of being a provider of choice for world-class photon sciences and facilities.

Steve Dierker

Steve Dierker
Associate Laboratory Director for Photon Sciences

SCIENCE HIGHLIGHTS



In FY10, Photon Sciences staff and users published 893 articles in journals, conference proceedings, reports, books, dissertations, and patents. Almost 20 percent were published in premiere journals (those that have an impact factor of 6 or greater). The following highlights are representative of this extensive and diverse research, ranging from the creation of new catalysts for renewable energy production to the exploration of the inner workings of diseases like tuberculosis and cancer.

FY10 publication count

Publication Type	Total	Staff
Total Publications	893	110
Total Journals	747	84
Peer-Reviewed Journals	724	81
Peer-Reviewed Premier Journals	165	21
Conference Proceedings	68	18
Reports: Technical, Formal, Informal	2	2
Books / Book Chapters	18	4
Theses / Dissertations	51	0
Patents	7	2

Anti-cancer Agent Stops Metastasis in its Tracks

Like microscopic inchworms, cancer cells slink away from tumors to travel and settle elsewhere in the body. Now, researchers have found that new anti-cancer agents break down the looping gait these cells use to migrate, stopping them in their tracks.

The researchers, from Cornell University's Weill Cornell Medical College and Brookhaven National Laboratory, found that mice implanted with cancer cells and treated with the small molecule macroketone lived a full life without any cancer spread, compared with control animals, which all died of metastasis. When macroketone was given a week after cancer cells were introduced, it still blocked greater than 80 percent of cancer metastasis in mice.

These findings provide an encouraging direction for development of a new class of anti-cancer agents, the first to specifically stop cancer metastasis, which kills more than 90 percent of cancer patients.

Their work started in 2003, after researchers in Japan isolated a natural substance, dubbed migrastatin, that is the basis of many antibiotic drugs. The Japanese researchers noted that migrastatin had a weak inhibitory effect on tumor cell migration. Weill scientists and collaborators at the Memorial Sloan-Kettering Cancer Center then built migrastatin analogues — synthetic and molecularly simpler versions.

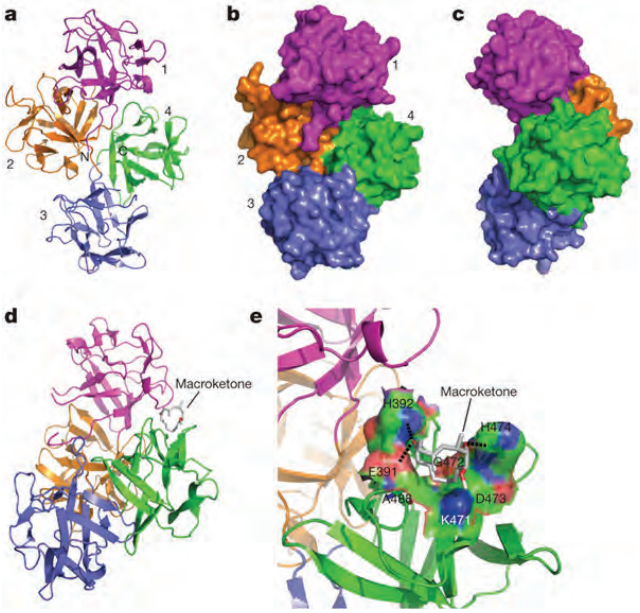
In 2005, they showed that several of the new versions, including macroketone, stopped cancer cell metastasis in laboratory animals, but they didn't know how the agent worked.

In the current study, the researchers used x-ray diffraction at NSLS beamlines X6A and X4C to reveal the mechanism. They found that macroketone targets a protein known as fascin that is critical to cell movement. In order for a cancer cell to leave a primary tumor, fascin bundles actin filaments together like a thick finger. The front edge of this finger creeps forward and pulls along the rear of the cell. Cells crawl away in the same way that an inchworm moves.

Macroketone latches on to individual fascin, preventing the actin fibers from adhering to each other and forming the pushing leading edge. Because individual actin fibers are soft when they are not bundled together, the cell cannot move.

— John Rodgers, Weill Cornell Medical College

L. Chen, S. Yang, J. Jakoncic, J.J. Zhang, X.-Y. Huang, "Migrastatin Analogues Target Fascin to Block Tumour Metastasis," *Nature*, **464**, 1062 (2010).



a) Structure of fascin shown as a ribbon diagram, viewed from the N-terminal and C-terminal plane. The four domains are colored magenta (1), orange (2), blue (3) and green (4). **b)** Surface presentation of fascin structure viewed in a. **c)** View of fascin turned clockwise 90 degrees along the *y* axis relative to the view in b. **d)** Overall structure of the complex of fascin and macroketone. The macroketone molecule is shown as a white stick model. **e)** Macroketone-binding site. Residues involved in interactions with macroketone are shown as surface, and hydrogen bonds are shown as dashed lines.

Accessing the Risk of Arsenic Ingestion with Mineralogy

Canadian researchers working at NSLS created a method for determining how much of the arsenic in soil tailings — byproducts of the mining industry — will enter the bloodstream if ingested.

In order to ensure that harmful mining waste is properly dealt with, it is important to determine how much of an ingested chemical is absorbed by the body rather than passed harmlessly through the digestive system. Scientists can approximate this as the chemical's bioaccessibility. Instead of feeding samples to a test subject, a bioaccessibility test runs the sample through conditions that simulate a digestive system, complete with mock gastrointestinal fluids. The percentage of arsenic that dissolves during this process reveals the sample's bioaccessibility.

But instead of running these tests on numerous soil samples from throughout a mining site, the researchers sought to describe the relationship between a sample's bioaccessibility and the specific minerals in it — its mineralogy. The researchers, from the Royal Military College of Canada, Queen's University, the British Geological Survey, and Geological Survey of Canada, examined soil samples taken in the gold mine districts of Nova Scotia, Canada, to try to predict, given the mineralogy of a sample, whether it's highly bioaccessible.

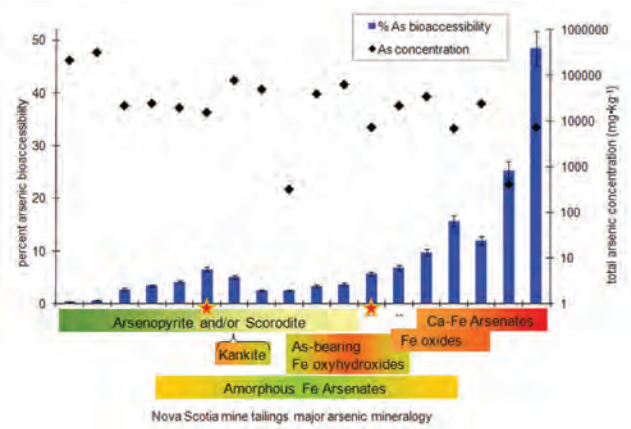
The research team tested the samples' mineralogy using micro-x-ray fluorescence and diffraction imaging techniques at NSLS and x-ray absorption near-edge structure analysis at Argonne National Laboratory's Advanced Photon Source.

Next, researchers compared the mineralogical results from NSLS with the samples' bioaccessibility, and found some interesting connections.

Single arsenic minerals, such as arsenopyrite, had lower bioaccessibility — over 90 percent of the arsenic in the sample would pass through the digestive system without being absorbed by the body. This is due to arsenopyrite's low solubility, or ability to dissolve in fluid. A more soluble compound, arsenic bearing iron(oxy)hydroxides, had 10 times the bioaccessibility of arsenopyrite.

But their findings don't mean that the old bioaccessibility tests should be eliminated. For example, certain compounds can increase the bioaccessibility of the entire soil sample surrounding it. Despite knowing the bioaccessibility of the minerals in the sample, researchers still need a bioaccessibility test of the entire sample to reveal its higher-than-expected toxicity.

L. Meunier, S.R. Walker, J. Wragg, M.B. Parsons, I. Koch, H.E. Jamieson, K.J. Reimer, "Effects of Soil Composition and Mineralogy on the Bioaccessibility of Arsenic from Tailings and Soil in Gold Mine Districts of Nova Scotia," *Environ. Sci. Technol.*, **44**, 2667 (2010).



Right: Lead researcher Kenneth Reimer, director of the environmental sciences group at the Royal Military College of Canada

Left: Mineralogy, percent arsenic bioaccessibility and total arsenic concentration of samples from Nova Scotia mine tailings. Detailed mineralogical analyses of individual samples revealed up to seven arsenic species in individual samples (six shown here as major arsenic phases). Results of a physiologically based extraction test are for the < 150 μm particle size fraction. A weak correlation is observed between total and bioaccessible arsenic concentrations. The percent arsenic bioaccessibility is most influenced by the presence of a more soluble arsenic species, even in low concentrations. Lower percent bioaccessibility in the majority of samples is associated with sparingly soluble arsenopyrite and scorodite. Higher percent bioaccessibility in some samples is attributed to the presence of calcium-iron arsenates and arsenic-bearing iron oxides. The star denotes the presence of a minor calcium-iron arsenate phase.

Reducing Penalties for Creating Block Copolymer Nanostructures

How do you make a material that has the elasticity of a rubber band and the thermal insulation of a Styrofoam cup? Connect two distinct polymer chains – poly(isoprene) and poly(styrene) – end to end like a series of children's building blocks. The result is an appropriately named "block copolymer" that boasts the properties of both materials and is commonly used in the tires of automobiles and the soles of athletic shoes.

But the most impressive trait of a block copolymer is its ability to self-assemble. Imagine, for example, dropping a mixture of poly(isoprene) and poly(styrene) on the floor. The two incompatible blocks will "phase separate" like oil and water. However, connect the ends of the two polymers together and the material usually can assemble into a well-defined material with nanoscale structure.

This natural assembly is extremely valuable for emerging nanoscale applications, including materials for fuel cells, lithium ion batteries, and organic photovoltaics.

In order to take full advantage of a block copolymer's molecular architecture, researchers are looking for ways to control the interactions between polymer blocks through means such as high temperatures and selective solvents.

To do this, University of Delaware researchers are exploring tuning with tapering, which increases the compatibility of the polymer by smoothing out the chemical interface between the two blocks.

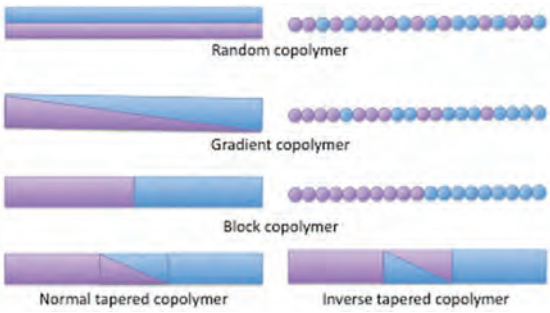
Tapering the interface is thought to reduce the "penalty" of mixing between the two very different blocks. The result is a lower processing temperature, which is easier and cheaper to achieve, and greater chemical compatibility.

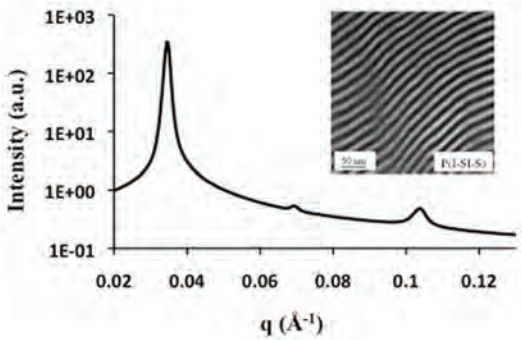
To test this idea, the researchers synthesized a number of tapered poly(isoprene-*b*-styrene) block copolymer samples at the University of Delaware: samples with different taper lengths (from 15-35 percent tapered material) with either normal or inverse tapering.

The samples were then heated and cooled while researchers observed the changes in the material with small-angle x-ray scattering at NSLS and Argonne's Advanced Photon Source, and transmission electron microscopy and dynamic mechanical analysis at the University of Delaware.

Their results proved that researchers can tune the compatibility of block copolymers (via tapering) with no detriment to the ordering or mechanical properties of the material. The research also revealed that inverse tapering gives the greatest increase in compatibility.

N. Singh, M.S. Tureau, T.H. Epps, III, "Manipulating Ordering Transitions in Interfacially Modified Block Copolymers," *Soft Matter*, **5**, 4757 (2009).





Left: University of Delaware researchers Thomas Epps (left) and Maeva Tureau

Right top: Cartoon of density profile and segment distribution along model polymer chains as a function of position, where purple represents isoprene and blue represents styrene, illustrating the difference between random, gradient, block, and tapered block copolymers.

Right bottom: Synchrotron-SAXS data for a P(I-SI-S) tapered diblock copolymer. Specimens were annealed at 210 degrees C and then cooled to room temperature for data acquisition. The integral moduli values are characteristic of two-domain lamellae. The inset shows a transmission electron microscopy image of a P(I-SI-S) specimen. The sample is stained by OsO_4 vapor to enhance contrast.

Clocking Ultra-fast Electron Bunches

Brookhaven researchers have developed a device that acts like a high-tech stopwatch for speedy packs of electrons just trillionths of a second long. This new diagnostic tool could aid in the development of x-ray free electron lasers (FEL), sources that produce pulses of light up to one billion times brighter and 1,000 times shorter than those produced at conventional storage ring light sources.

Like a high-speed strobe light, the ultra-short bursts of light produced from an FEL allow scientists to take stop-motion pictures of chemical reactions, biological processes, and various other atomic-scale events. FELs create this valuable x-ray light by shooting a series of ultra-short bunches of electrons through an array of specialized magnets. The shorter the electron bunches, the more powerful the resulting light.

In recent years, the bunch lengths of electrons in accelerators have decreased dramatically, producing extremely bright pulses of light that are on the same time scale as vibrations in molecules and the creation or breakage of chemical bonds. But in order to synchronize the time-dependent process being studied with the x-ray pulse, scientists need new beam diagnostics capable of measuring the length of picosecond-scale (one millionth of one millionth of a second) pulses.

At the NSLS Source Development Laboratory (SDL), Brookhaven researchers have demonstrated a high-resolution measurement system that's nondestructive to the electron beam and can be easily transported among facilities.

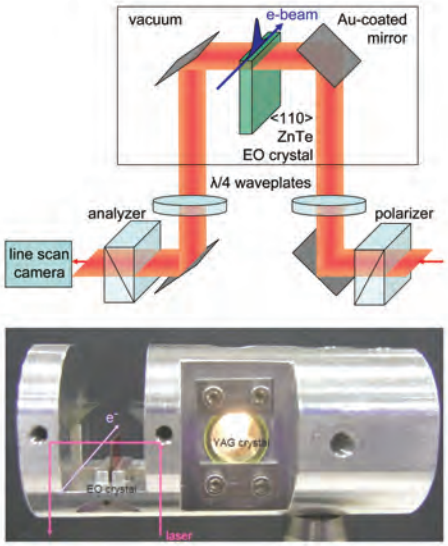
In the setup (first proposed by Brookhaven researchers in 2002), a beam of electron bunches is sent across the top edge of a thin, "electro-optical" crystal. Traveling at close to the speed of light, each electron bunch emits an electric field that travels downward through the crystal. At the same time, a single, line-focused laser pulse is sent straight through the broad side of the crystal, where sections of the laser line are encoded with spatial information from the electron bunches. A special camera at the end of the device collects these data.

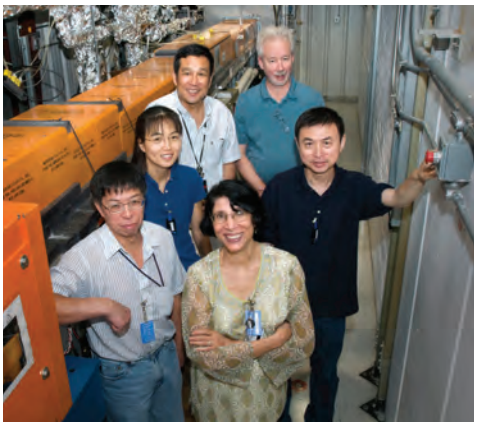
Now, the goal is to measure electron pulses an order of magnitude smaller, in femtosecond duration, or quadrillionth of a second range.

X. Yang, T. Tsang, T. Rao, J.B. Murphy, Y. Shen, X.J. Wang, "Electron Bunch Length Monitors Using Spatially Encoded Electro-Optical Technique in an Orthogonal Configuration," *Appl. Phys. Lett.*, **95**, 231106 (2009).

Left: (top) Schematic layout of the electro-optical arrangement. (bottom) The electro-optical module with a YAG crystal for electron beam position monitor.

Right: Clockwise from front: Triveni Rao, Thomas Tsang, Xi Yang, Xijie Wang, Jim Murphy, and Yuzhen Shen





DNA Repair Changes with the Flip of a Switch

The DNA blueprint in each human cell undergoes about 100,000 damaging events every day. Because a cell's survival depends on the repair of these damaged molecules, each injury signals a team of proteins to work together to fix the mutated DNA.

In pursuit of a better fundamental understanding of DNA repair, researchers from the National Institute of Environmental Health Sciences use NSLS to image a large, multi-part molecule called a scaffolding protein. The molecule, XRCC1, orchestrates DNA repair by holding the other repair proteins together in a multi-molecule complex.

A technique called SAXS, for small-angle x-ray scattering, allows the researchers to take a low-resolution picture of the molecule, obtaining a macroscopic image rather than the details of its fine structure. In SAXS, a protein in solution (the state in which it exists in the body) can be targeted with x-rays, which then scatter and hit a detector, allowing researchers to reconstruct an image of the protein's surface.

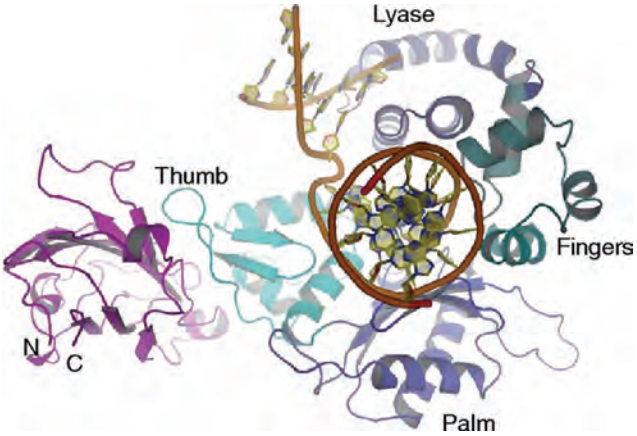
Using SAXS, the researchers studied a subsection of XRCC1 called the N-terminal domain. The N-terminal domain interacts with DNA polymerase β, a protein that actively repairs damaged DNA. Their study shows that this interaction can change with the flick of a biological switch.

The N-terminal domain contains a "disulfide switch," a potential bond whose formation changes the molecule's secondary structure. When the bond forms, the switch is flipped on, transforming the molecule from a reduced state to an oxidized state. In the reduced state, one of the amino acids that make up the N-terminal domain has electrons to spare. This makes the amino acid very susceptible to oxidation, a process in which it shares these electrons with another amino acid, forming a disulfide bond between the electron sharer and receiver and transforming the N-terminal domain into its oxidized state.

In this case, the oxidized surface binds more strongly to DNA polymerase β than does the surface of the reduced form.

Discovering the disulfide switch's role would help improve scientists' understanding of how DNA repair works, knowledge that could lead to better treatments for disease.

M.J. Cuneo, R.E. London, "Oxidation State of the XRCC1 N-terminal Domain Regulates DNA Polymerase β Binding Affinity," *PNAS*, **107** (15), 6805 (2010).



Top: Model of the complex formed by XRCC1's N-terminal domain (in purple), damaged DNA (in orange), and DNA polymerase β (with component parts thumb, lyase, fingers, and palm labeled).

Bottom: Matthew Cuneo (left) and Robert London (photo courtesy of Steven R. McCaw, Image Associates)

Cracking the Children's Fingerprint Disappearing Act

Children's fingerprints disappear faster than those of adults — a little-known fact that can hamper investigations of kidnapping cases. To investigate this phenomenon, a team of researchers used beams of infrared light at NSLS as a powerful detective's microscope, finding that fingerprint staying power is based on the amount and types of oil in your skin.

Forensic scientists often use techniques like magnetic filings dusting, iodine, and cyanoacrylate fuming to see otherwise invisible, or latent, fingerprints. Although efficient, inexpensive, and relatively fast, these methods make it difficult to preserve trace evidence found in a fingerprint.

Previous research has linked the difference in the longevity of fingerprints to the type of oil found in a person's skin. This oil, known as sebum, is just one of the components of a fingerprint, which also can contain small pieces of skin and sweat residue. The NSLS researchers wanted to determine how these fingerprint components change over time in adults and children.

Using a collection of latent fingerprints given by father and son pairs, the researchers watched for chemical changes over the course of four weeks. Twice a week, one fingerprint from each participant was dusted, lifted, and analyzed based on the number of features, or minutiae, visible. At the same time, a non-invasive synchrotron technique called Fourier transform infrared microspectroscopy (FTIRM) mapped the location and makeup of the skin and sebum in the prints.

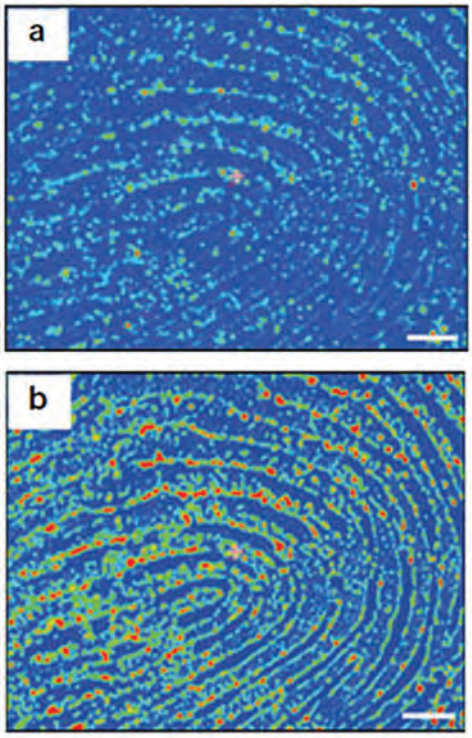
At all points in time, the fathers' prints dusted darker than those from their sons, remaining virtually unchanged during the study, while the fine minutiae of their children became increasingly more difficult to see.

As predicted by previous studies, FTIRM showed that adults produce more sebum than children, which leads to darker prints. Researchers also found that the composition of the lipids, or fats, in sebum differ significantly between adults and children.

Adult sebum has higher concentrations of stable lipids such as squalene and wax esters, which are less likely to vaporize over time. Conversely, the sebum of children contains higher levels of cholesterol and branched chain free fatty acids — unstable lipids that break down more quickly.

The results could pave the path toward more advanced fingerprint detection techniques.

K.M. Antoine, S. Mortazavi, A.D. Miller, L.M. Miller, "Chemical Differences are Observed in Children's Versus Adults' Latent Fingerprints as a Function of Time," *J. Forensic Sci.*, **55**(2), 513 (2010).



Left: FTIRM images generated from a child's fingerprint, showing the **a)** protein in the fingerprint, and **b)** the oil (sebum) in the print.

Right: Lead author Kimone Antoine

The Molecular Mechanics of Hearing and Deafness

Our senses are essential for survival and for the exploration of natural environments, and much has been learned about the molecular basis of vision, olfaction, and taste. Yet only a few of the molecules mediating touch and sound perception have been discovered.

Now, researchers from Harvard University have resolved the molecular structure of one key protein important for sound perception. They used this structure, together with molecular dynamics simulations, to understand the protein's mechanics and function in hearing and deafness.

Hair cells of the inner ear are exquisite mechanoreceptors: minute motion of their apical hair bundles by sound becomes an electrical signal that is then transmitted to the brain. At the core of this mechanotransduction process there is a fine filament — termed the "tip link" — that pulls open force-gated ion channels, thereby causing depolarization. This tip link filament is made of two atypical cadherins, cadherin-23 and protocadherin-15. Mutation of either causes hereditary deafness.

To elucidate the function of these proteins, the researchers determined the x-ray crystal structure of cadherin-23's N-terminal end at the Advanced Photon Source at Argonne National Laboratory and NSLS. The structure revealed a novel calcium binding site that defines a subfamily of cadherin adhesion molecules.

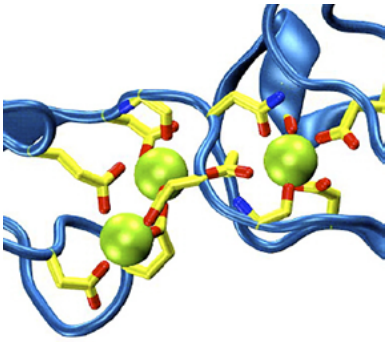
Classical cadherins, the calcium-dependent "glue" that keeps cells together in multicellular organisms, use a "strand-exchanged" mechanism to form adhesive bonds. However, the new structure suggests that cadherin-23 must use a different mechanism, perhaps through a calcium bridge, with calcium ions participating in the interface between cadherin-23 and protocadherin-15.

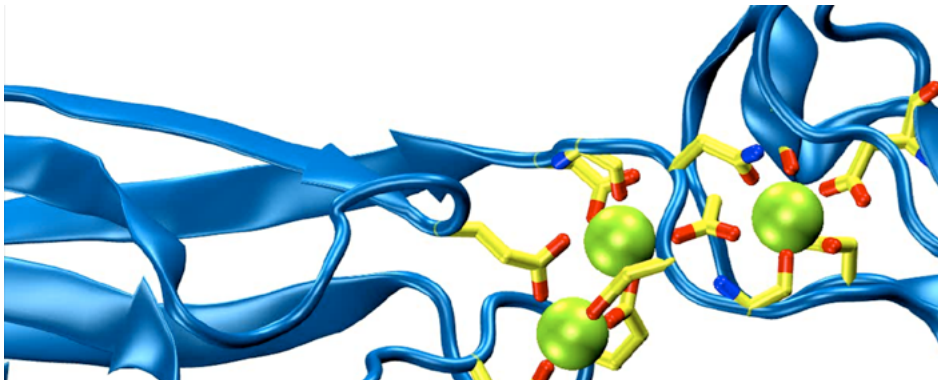
With the cadherin-23 structure in hand, the team used molecular dynamics simulations to determine its elasticity. The tip link has been assumed to be a relatively elastic, spring-like molecule. However, an extensive set of atomistic simulations revealed a stiff cadherin-23 molecule, with tightly-bound calcium ions preventing mechanical unfolding.

Structural information on wild-type and mutant cadherin-23 proteins can help pinpoint the mechanisms by which mutations cause disease. The team used the determined crystal structure of cadherin-23 carrying a mutation known to cause deafness in humans. Biochemical assays demonstrated that this mutation impairs calcium binding, and simulations showed that in the absence of bound calcium, cadherin-23 becomes a mechanically weak protein. The mutation-induced weakening of cadherin-23 suggests that mutant tip links are more prone to mechanical failure, causing hearing loss.

— David Corey and Rachelle Gaudet, Harvard University

M. Sotomayor, W.A. Weihofen, R. Gaudet, D.P. Corey, "Structural Determinants of Cadherin-23 Function in Hearing and Deafness," *Neuron*, **66**(1), 85, (2010).





Top: A close-up view of the linker region between cadherin-23 repeats 1 and 2 is shown while the protein is stretched from both ends. The simulation mimics in vivo conditions in which tip-link cadherins are stretched during sound mechanotransduction at hair cells of the inner ear. Calcium ions (shown as green spheres) were found to be essential for the mechanical stability of the protein (shown in cartoon and sticks).

Bottom: Click image to view simulation movie

Brown-led Research Divines Structure for Class of Proteins

Most proteins are shapely, but about one-third of them lack a definitive form, at least that scientists can readily observe. These intrinsically disordered proteins (IDPs) perform a host of important biological functions, from muscle contraction to other neuronal actions. Yet despite their importance, scientists don't know much about them.

Now, researchers at Brown University, the University of Toronto, and Brookhaven National Laboratory have discovered the structure of three IDPs — spinophilin, I-2, and DARPP-32. Besides getting a handle on each protein's shape, the scientists presented for the first time how these IDPs exist on their own (referred to as "free form") and what shape they assume when they latch on to protein phosphatase 1, known as "folding upon binding."

Determining the IDPs' shape gives molecular biologists insight into what happens when IDPs fold and regulate proteins, such as PP1, which must occur for biological instructions to be passed along.

For two years, the researchers used a variety of techniques to ascertain each IDP's structure. With I-2, which instructs cells to divide, they used nuclear magnetic resonance spectroscopy to create ensemble calculations for the protein in its free and PP1-bound form. They confirmed I-2's binding interaction with PP1 with the help of small-angle x-ray scattering measurements at NSLS.

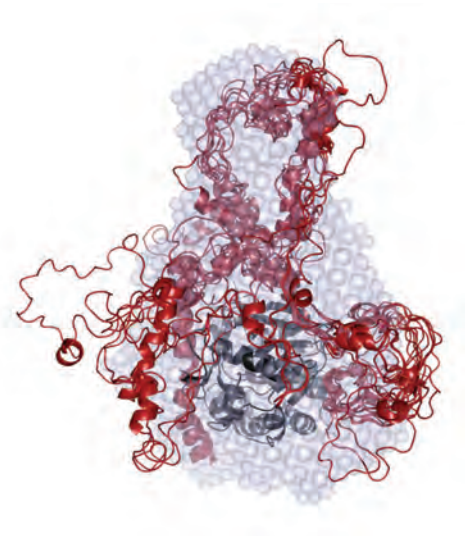
The researchers did the same thing to determine the structure of spinophilin and DARPP-32 in their free-form state and to gain insights into their shapes when they bind with PP1.

— Richard Lewis, Brown University

J.A. Marsh, B. Dancheck, M.J. Ragusa, M. Allaire, J.D. Forman-Kay, W. Peti, "Structural Diversity in Free and Bound States of Intrinsically Disordered Protein Phosphatase 1 Regulators," *Structure*, **18**(9), 1094, (2010).

Left: Researchers used a variety of experimental, mathematical and observational techniques to ascertain how I-2, one of a class of poorly understood proteins known as intrinsically disordered proteins, binds with the regulator protein phosphatase 1.

Right: Lead researcher Wolfgang Peti, associate professor of medical science and chemistry at Brown University



A Hidden Magnetic Configuration in Manganite Thin Films

Complex oxide materials are intriguing because their properties span an enormous range of distinct physical states, including conductors, insulators, superconductors, ferromagnets, anti-ferromagnets, ferro-electrics, piezo electrics, and multiferroics. Part of the attraction of these materials is that their properties can be modified by introducing a mixed valence state — that is, a composition that includes metal ions with more than one oxidation state.

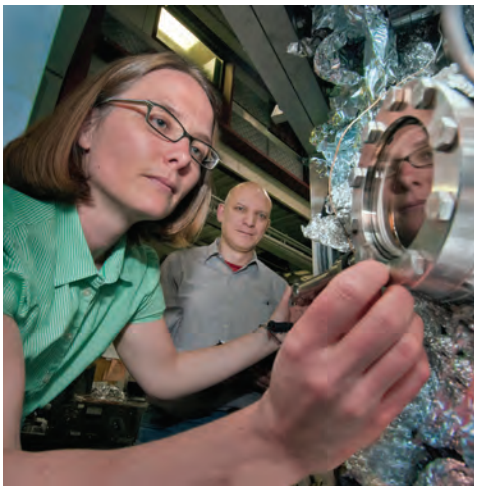
Scientists from Brookhaven and Lawrence Berkeley national laboratories, SLAC National Accelerator Laboratory, and collaborators at the University of California, Berkeley, and the Science and Technology Facilities Council of the UK are taking a closer look at one such material with a particular composition of lanthanum strontium and magnesium oxide.

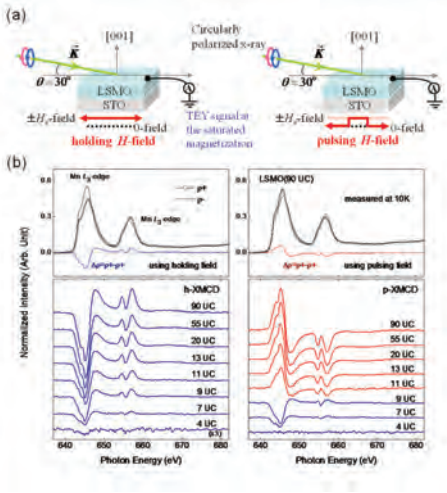
$La_{0.7}Sr_{0.3}MnO_3$ (LSMO) is a mixed-valence, complex oxide (containing a mix of Mn^{3+} and Mn^{4+} ions) whose properties have been examined extensively. LSMO is thought to be a simple metallic ferromagnet and it has been used in prototype, thin-film electrical devices (such as magneto-resistance junctions) that seek to exploit the many intriguing properties of complex oxides for new applications.

To further explore LSMO, the scientists grew single-layer films with a variable number of unit cells epitaxially on strontium titanate (STO). Using a combination of x-ray magnetic circular dichroism, x-ray absorption spectroscopy, and x-ray reflectivity measurements at NSLS, the scientists discovered that, due to doping instabilities and/or charge transfer at the interface, an intermediate enriched Mn^{3+} layer of a few unit cells develops at the LSMO/STO interface. The presence of this intermediate layer may provide a mechanism for antiferromagnetic coupling across the interface — which, in turn, may lead to the reversed magnetic configuration observed in thicker LSMO films.

The findings demonstrate the rich variety of interfacial spin couplings that can occur in complex oxide thin films that may be utilized in engineering thin-film devices.

J.-S. Lee, D.A. Arena, P. Yu, C.S. Nelson, R. Fan, C.J. Kinane, S. Langridge, M.D. Rossell, R. Ramesh, and C.-C. Kao, "Hidden Magnetic Configuration in Epitaxial $La_{1-x}Sr_xMnO_3$ Films," *Phys. Rev. Lett.*, **105**, 257204, (2010).





Left: NSLS researchers Christie Nelson (left) and Dario Arena

Right: (a) Schematic picture of experimental configurations for *h* x-ray magnetic circular dichroism (XMCD) (left) and *p* XMCD (right). **(b)** Thickness dependent XMCD results on LSMO at T=10 K. Left is *h* XMCD. Right is *p* XMCD.

An Elegant Cycle: Molybdenum's Availability in Soil Deciphered

Researchers from Princeton University working at NSLS have solved the mystery of how molybdenum, one of the elements needed to prepare nitrogen for plant consumption, is available in soil.

Nitrogen is key to cellular growth and the functioning of proteins and nucleic acids in plants and other organisms. Pure nitrogen molecules are plentiful in the atmosphere, but their atmospheric form is not usable by most organisms. Nature's solution is a process called nitrogen fixation, in which nitrogen is combined with hydrogen or oxygen to create a new molecule that can be used by various organisms.

Molybdenum is one of the elements needed to jump-start nitrogen fixation. Until now, scientists haven't entirely understood how molybdenum is present and available in the soil to become a catalyst.

To solve this mystery, Princeton scientists collected samples from molybdenum-rich Arizona soil and a temperate hardwood forest in New Jersey.

After some initial troubleshooting at the Stanford Synchrotron Radiation Lightsource, they brought their samples to NSLS to map out, on the micro-scale, how molybedenum is distributed and in what form, as well as how it adheres to other minerals.

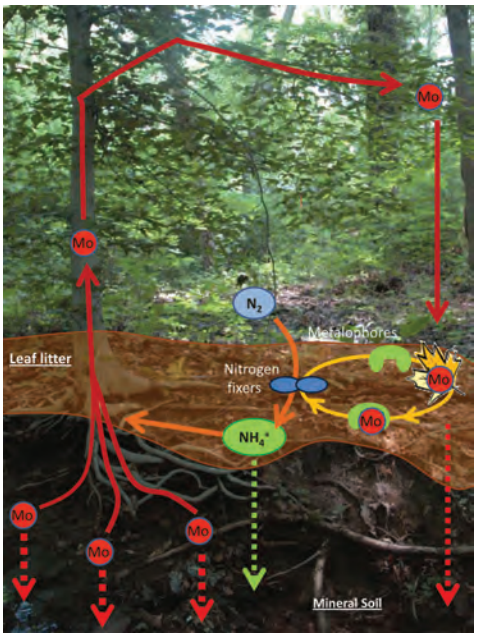
Consistent with past observations, molybdenum was found to stick to the surfaces of iron oxides. But the scientists also found strong evidence of molybdenum binding to natural organic matter, particularly in the upper soil layers, rich in leaf-litter and free-living nitrogen-fixing bacteria.

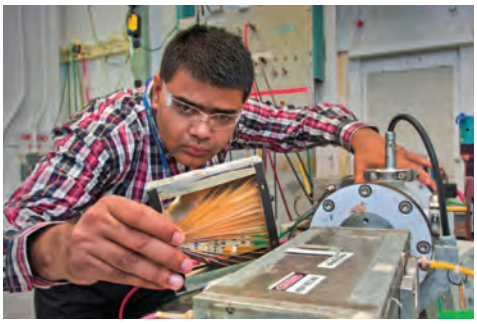
This finding suggests a molybdenum cycle: molybdenum in the soil is taken up by tree roots and deposited in leaves. These leaves fall to the ground and decompose, releasing molybdenum, which binds to tannins and tannin compounds in soil.

To understand how molybdenum transforms into a catalyst for nitrogen fixation, the researchers studied the nitrogen-fixing bacteria in soil with tannin-bound molybdenum. They found that the bacteria excrete a compound that strongly attracts iron and other metals. Molybdenum, held in the upper soil by tannin, binds to this compound, which can outcompete the tannin in attracting molybdenum. This new molybdenum compound is one that nitrogen-fixing bacteria can access to create the enzyme responsible for nitrogen fixation.

In turn, fixed nitrogen will penetrate the soil, be taken up by the root system of plants and promote plant growth.

T. Wichard, B. Mishra, S.C. Myneni, J-P Bellenger, A.M.L. Kraepiel, "Storage and Bioavailability of Molybdenum in Soils Increased by Organic Matter Complexation," *Nature Geoscience*, **2**, 625-629 (2009).





Left: The molybdenum (Mo) cycle in soil: Mo present in deep soil is extracted by the root network of trees and incorporated into leaves. These leaves fall to the ground and decompose, providing a Mo-enriched environment for nitrogen-fixing bacteria living in the upper soil. Binding of Mo to leaf organic matter reduces Mo leaching rates from the soil, keeping Mo in the soil environment where it can be used by the bacteria. In turn, the new nitrogen fixed by the bacteria fertilizes tree growth, resulting in a classic mutualistic relationship.

Right: Corresponding author Bhoopesh Mishra (now at Argonne National Laboratory), who conducted this study as a post-doc at Princeton University

Scientists Glimpse Nanobubbles on Super Non-Stick Surfaces

Non-stick surfaces are important to many areas of technology, from drag reduction to anti-icing agents. These surfaces are usually created by applying coatings, such as Teflon, to smooth surfaces. But recently, scientists have realized that a bit of texture can help. By incorporating topographical features on surfaces, they've created extremely water-repellant materials.

This effect, called "superhydrophobicity," occurs when air bubbles remain trapped in the textured surfaces, drastically reducing the area of liquid in contact with the solid. As a result, water is forced to ball up into pearl-shaped drops, which are weakly connected to the surface and can readily roll off.

To get the first look at nanobubbles on a superhydrophobic surface, the scientists created a regular array of more than a trillion nano-cavities on an otherwise flat surface, and then coated it with a wax-like surfactant at Brookhaven's Center for Functional Nanomaterials.

This coated, nanoscale-textured surface was much more water repellant than the flat surface alone, suggesting the existence of nanobubbles. To prove that these ultra-small bubbles were present, the researchers took transmission small-angle x-ray scattering measurements at NSLS beamline X6B.

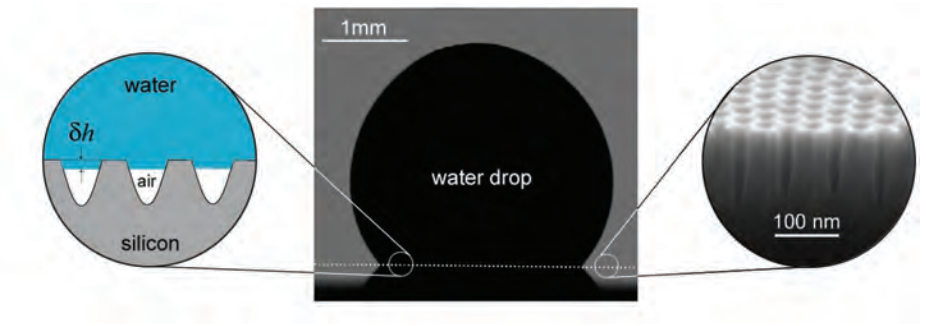
They found that the cavities were mostly filled with air, with water penetrating only about 5 to 10 nanometers into the cavities, independent of their depth. This provides the first direct evidence of the morphology of such small bubbles.

The researchers' results also show that the bubbles are only about 10 nanometers in size — about 10,000 times smaller than the width of a single human hair — and have nearly flat tops.

In contrast to materials with larger, micrometer-sized bubbles (which have rounded tops), the surfaces fabricated by the Brookhaven-led team may exhibit more stable superhydrophobic properties.

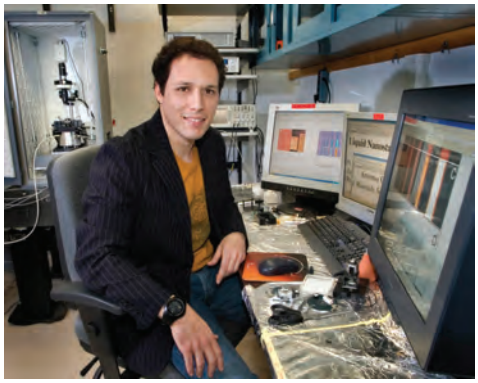
The research could lead to a new class of non-stick materials for a range of applications, including improved-efficiency power plants, speedier boats, and surfaces that are resistant to contamination by germs.

A. Checco, T. Hofmann, E. DiMasi, C.T. Black, B.M. Ocko, "Morphology of Air Nanobubbles Trapped at Hydrophobic Nanopatterned Surfaces," *Nano Lett.*, **10**(4), 1354 (2010).



Top: In this picture, the central image is the optical profile of a water drop placed on "nanopitted" silicon; the right image is a scanning electron micrograph of the nanocavities; and the left image is a cartoon illustrating the nanobubbles' shape as inferred from x-ray measurements.

Bottom: Brookhaven physicist Antonio Checco



Water-splitting Photocatalyst Brought to Light

To produce "green" fuels, some scientists are looking for a little help from above. Sunlight is the key ingredient in photocatalytic water splitting, a process that breaks down water into oxygen and, most importantly, hydrogen, which could be used in future energy technologies like fuel cells. The problem is that the most effective photocatalysts, like pure titanium dioxide, are only activated by ultraviolet light.

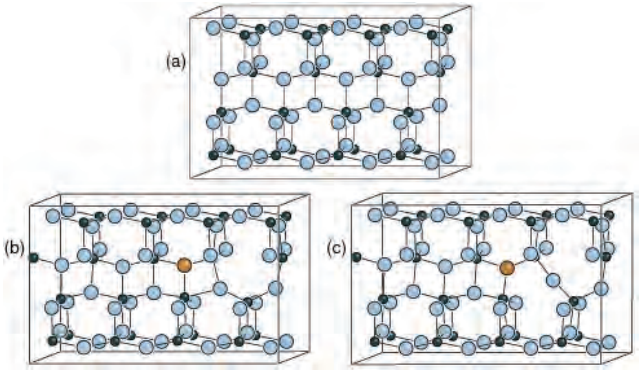
Recently, scientists have found a way alter titanium dioxide to react to visible light, harnessing the power of the entire solar spectrum. They do this by adding, or "doping," a small amount of nitrogen to titanium dioxide.

At NSLS, scientists from Brookhaven, the National Institute of Standards and Technology (NIST), and the University of Delaware set out to reveal what's so special about the doped form of the material.

The group analyzed samples made at the University of Delaware with hard x-ray photoelectron spectroscopy (HAXPES) studies at NSLS beamline X24A – the only facility in the United States that performs this advanced technique. HAXPES allows researchers to probe the electronic structure of materials deeper than regular photoemission studies, which are usually limited to surfaces. By combining these data with calculations carried out by the theory group at NIST, the researchers discovered that the addition of nitrogen changed the electronic structure both directly and indirectly.

Their findings: by adding nitrogen to the material, a certain amount of oxygen is forced out. The resulting oxygen vacancy, combined with the presence of nitrogen itself, explains the observed electronic structure.

A.K. Rumaiz, J.C. Woicik, E. Cockayne, H.Y. Lin, G. H. Jaffari, and S.I. Shah, "Oxygen Vacancies in N Doped Anatase TiO_2: Experiment and First-principles Calculations," *Applied Physics Letters*, **95**, 262111 (2009).



Left: (a) Structure of pure anatase, **(b)** $N/Ti^{3+}/O$ vacancy defect complex with O opposite N, **(c)** "Merging" of two O into central position. In (b) and (c), the Ti^{3+} ion is obscured from this viewpoint.

Right: Researchers Abdul Rumaiz (left) and Joe Woicik

Multi-Component Nano-Structures with Tunable Optical Properties

Scientists at Brookhaven National Laboratory report the first successful assembly of 3-D multi-component nanoscale structures with tunable optical properties that incorporate light-absorbing and -emitting particles. This work, using synthetic DNA as a programmable component to link the nanoparticles, demonstrates the versatility of DNA-based nanotechnology for the fabrication of functional classes of materials, particularly optical ones, with possible applications in solar-energy conversion devices, sensors, and nanoscale circuits.

Like earlier work conducted by the research team, this technique makes use of the high specificity of binding between complementary strands of DNA to link particles together in a precise way.

In the current study, the DNA linker molecules had three binding sites. The two ends of the strands were designed to bind to complementary strands on "plasmonic" gold nanoparticles — particles in which a particular wavelength of light induces a collective oscillation of the conductive electrons, leading to strong absorption of light at that wavelength. The internal part of each DNA linker was coded to recognize a complementary strand chemically bound to a fluorescent dye molecule. This setup resulted in the self-assembly of 3-D body centered cubic crystalline structures with gold nanoparticles located at each corner of the cube and in the center, with dye molecules at defined positions in between.

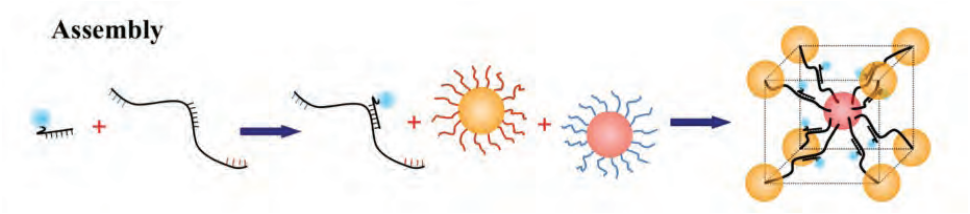
The scientists also demonstrated that the assembled structures can be dynamically tuned by altering the salt concentration of the solution in which they are formed. Changes in salinity alter the length of the negatively charged DNA molecules, leading to reversible contraction and expansion of the whole lattice by about 30 percent in length.

The expansion and contraction of the crystal lattice allowed for a dramatic modulation of an optical response: a three-fold increase in the emission rate of the fluorescent molecules was observed.

These results were determined using a combination of small angle x-ray scattering at NSLS and time-resolved fluorescent methods at the CFN.

An understanding of these interactions could be relevant for developing novel optical materials for photovoltaic, photocatalysis, computing, and light-emitting applications.

H. Xiong, M.Y. Sfeir, O. Gang, "Assembly, Structure, and Optical Response of Three-Dimensional Dynamically Tunable Multi-component Superlattices," *Nano Letters*, **10**(11), 4456 (2010).



Top: Brookhaven scientists used DNA linkers with three binding sites (black "strings") to connect gold nanoparticles (orange and red spheres) and fluorescent dye molecules (blue spheres) tagged with complementary DNA sequences. These units are self-assembled to form a body-center cubic lattice with nanoparticles at the corners and in the center, and fluorescent dye molecules in between.

Bottom: Brookhaven Lab researcher Oleg Gang

Researchers Find Way to "See" Water Molecules Hidden Inside Proteins

A team of researchers from Case Western Reserve University has discovered a way to look at water molecules hidden deep inside proteins, revealing a network through which information flows when proteins are switched "on."

The team looked inside rhodopsin, the protein found in the retina at the back of the eye that is responsible for dim light perception. Rhodopsin is a member of a group of proteins called the G-protein coupled receptor (GPCR) superfamily, which physically change shape when turned "on," leading to interactions with other proteins and sending information across cell membranes to regulate many important molecular pathways. Rhodopsin is switched on by light, causing it to change shape and start a series of molecular events that make night vision possible.

The research team combined two techniques to investigate water's role in the protein's shape shifting. With radiolytic protein footprinting at NSLS beamline X28C they created hydroxyl radicals from the water molecules, which then chemically modify nearby amino acids inside the protein.

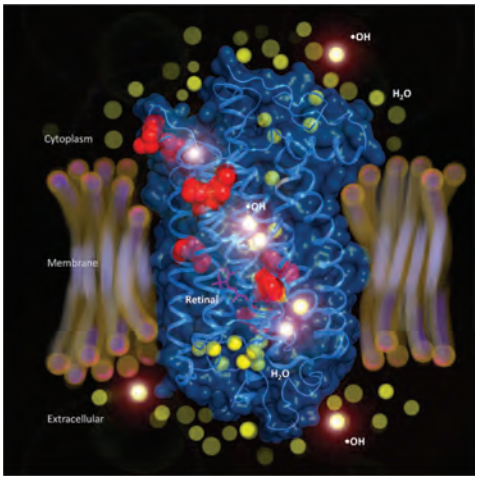
The researchers detected the chemical modifications using mass spectrometry and created molecular maps showing where water molecules sit inside the protein when it was off and on. They found that the water molecules rearranged in response to the protein being turned on and interacted with key areas necessary for the protein's function.

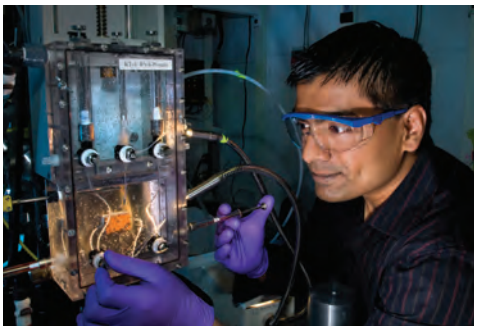
Specifically, water makes an electrostatic network within the proteins, which mediates the flow of information from one side of the protein to the other across the cell membrane.

Genetic mutations within the regions of the protein found to associate with water are known to cause diseases. For example, mutations in these areas of the rhodopsin protein cause a type of genetic night blindness that often leads to complete vision loss. GPCRs are also the gatekeepers that jumpstart many other biological responses, such as the flight or fight response, mood, and even heart function.

If scientists can learn how to turn these proteins and signaling pathways on and off, they can make a large-scale impact on biological response.

T.E. Angel, S. Gupta, B. Jastrzebska, K. Palczewski, M.R. Chance, "Structural Waters Define a Functional Channel Mediating Activation of the GPCR Rhodopsin," *PNAS*, **106** (34), 14367-72 (2009).





Left: Radiolytic footprinting of the membrane bound G-protein coupled receptor rhodopsin demonstrates the structural activation of bound waters as a function of receptor signaling status. X-rays ionize water molecules inside and outside the membrane protein structure to radicals (•OH, glowing spheres) that react with adjacent amino acid side chains. As the protein changes its structure during signaling, the pattern of reactivity of water within the protein changes reflecting the transmission of the signal through the membrane.

Right: Sayan Gupta, co-author of the study

A Straightforward Solution for Increasing Solar Cell Performance

An exciting development in the field of solar cells has been the discovery of organic semiconductors, which can, in principle, lower the manufacturing costs of large-area solar devices. But solar cells made from semiconducting organic materials, based on carbon, have their own drawbacks. Although this class of solar cells may provide a more cost-effective manufacturing route, they also are less efficient.

Solar cells made from organic plastic materials may deform a little bit when put out in the hot sun, and their electrical properties may change as they move. For solar cells made out of such materials to really work, they will need to withstand significant changes in conditions.

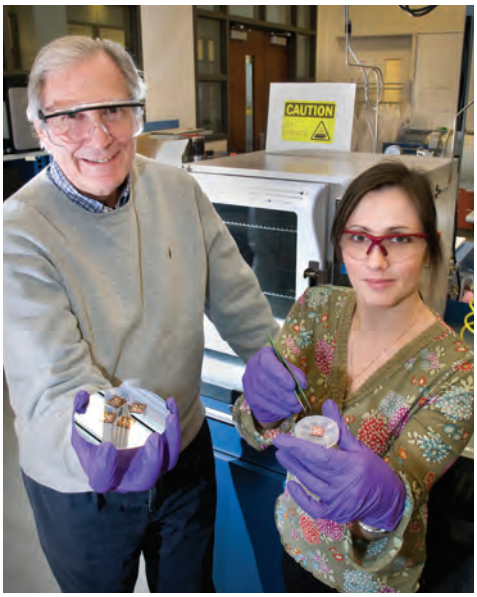
Researchers from Brookhaven Lab report that one way to increase the stability of organic solar cells is "locking" in place the semiconducting base layer, the first layer upon which the solar cell is built. To do this, a chemical crosslinker, which interconnects the polymer chains in the material's base layer, was added to the solution-based starting materials. This high degree of interconnection immobilizes the polymer structure and helps preserve its properties during changes in temperature, for example.

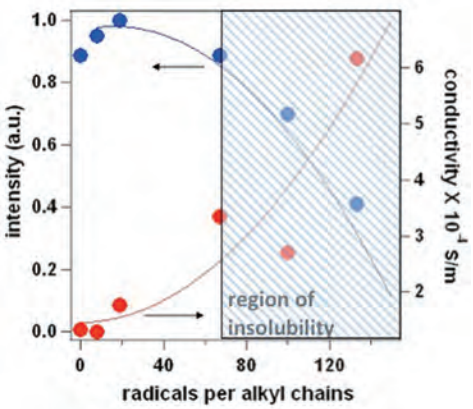
The crosslinker mechanically stabilizes the polymer and increases its conductivity by as much as five times. The efficiency of model solar cells made from the crosslinked polymer also increased, up to three fold. The solution-based process is cost-effective and allows for large-scale uses, such as in spray-on or roll-to-roll manufacturing methods.

Using x-ray diffraction at NSLS beamline X6B, the group investigated whether structural changes in the polymer film induced by crosslinking were related to the observed improvements in conductivity and device efficiency. The measurements showed that the polymer chains orient in such a way that electronic charge follows a more direct pathway through the film.

The new technique provides a way to create a stable polymer foundation upon which additional semiconducting materials can be layered — a necessary component of realizing more complex solar cell designs.

I.R. Gearba, C-Y Nam, R. Pindak, C.T. Black, "Thermal Crosslinking of Organic Semiconducting Polythiophene Improves Transverse Hole Conductivity," *Appl. Phys. Lett.*, **95**, 173307 (2009).





Left: Ioana Gearba (right), a former researcher at the CFN, and Ron Pindak, Physical and Chemical Sciences Division Head at NSLS, display the enhanced polythiophene blended solar cells.

Right: Properties of polythiophene polymer after crosslinking with radical initiator ditert butyl peroxide. The intensity of light absorption (blue circles) is unchanged with up to 70 radicals per alkyl chain of crosslinker. Conductivity (red circles) increases, up to five times, as increasing concentrations of crosslinker are added. The addition of 70 radicals per alkyl chain of crosslinker immobilizes the polymer, preserves its absorption properties, and increases conductivity by three times (shown by solid line).

'Super-catalyst' Found to Purify Hydrogen

Hydrogen — the lightest and most abundant element on the periodic table — is also a potential powerhouse. Today, we use pure hydrogen in a range of chemical processes, including the synthesis of ammonia for fertilizers. Some scientists believe that hydrogen could power everything from electronics to buildings to cars in a model referred to as the hydrogen economy. In order to achieve such feats, however, scientists need to produce pure hydrogen.

Chemists can obtain pure hydrogen through the water-gas shift reaction, in which carbon monoxide and water yield carbon dioxide and pure hydrogen molecules.

Four years ago, a group of Brookhaven-led researchers began to investigate a highly effective catalyst for this reaction, which combined gold and ceria. Their main objective was to understand exactly how each component of the catalyst behaved.

Beginning with this first catalyst, and gradually tweaking one variable after another, the researchers set out to find even better catalytic combinations. Using characterization techniques like photoemission, time-resolved x-ray diffraction and x-ray absorption spectroscopy at NSLS beamlines U7A, U12, X7B, and X19A, they studied details of the structural and electronic properties of the gold-ceria catalyst.

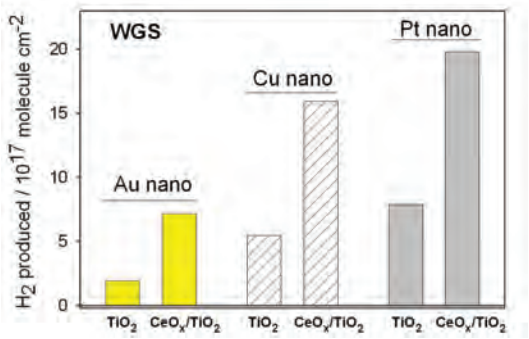
With in-situ characterization, researchers can determine two key factors: precisely when the active phase for the reaction appears on the catalyst and how it affects the reaction mechanism. These key factors allow scientists to refine the reaction, exchanging and adjusting its components.

Last year, the researchers tested a new catalyst that combines ceria in a mixed metal oxide, building upon the findings of their previous research. They found that this surface combination with a dispersion of gold, copper, or platinum nanoparticles revealed high catalytic properties.

More recently, they compared catalytic effects with a dispersion of gold, copper, and platinum nanoparticles. While platinum showed the highest catalytic activity, meaning it produced the most hydrogen for a fixed amount of ceria, copper was a close second and has the advantage of being a much less expensive metal.

Studying this next-generation catalyst could reveal more discoveries and lead to an even more potent super-catalyst.

J.B. Park, J. Graciano, J. Evans, D. Stacchiola. S.D. Senanayake, L. Barrio, P. Liu, J.F. Sanz, J. Hrbek, J.A. Rodriguez, "Gold, Copper, and Platinum Nanoparticles Dispersed on $CeO_x/TiO_2(110)$ Surfaces: High Water-Gas Shift Activity and the Nature of the Mixed-Metal Oxide at the Nanometer Level," *J. Am. Chem. Soc.*, **132**, 356 (2010).



Top: Production of hydrogen through the water-gas shift reaction after dispersing gold (Au), copper (Cu), and platinum (Pt) on $TiO_2(110)$ and the group's "super-catalyst," $CeO_x/TiO_2(110)$

Bottom: From left, Brookhaven researchers Sanjaya Senanayake, Jose A. Rodriguez, Laura Barrio, and Jonathan Hanson

Expanding the Toolbox for Superconducting Film Investigations

Using a combination of unique tools to build and analyze films just nanometers thick, a group of researchers found subtle structural changes that are known to alter superconducting properties. Their findings stress the importance of studying both the superficial and deep features of superconducting materials, which transport electricity with zero resistance and are envisioned for use in applications like ultrafast, power-saving electronics or more efficient electricity lines.

The study was spurred by a surprising discovery made in 2008 by a Brookhaven-led research team: an ultrathin film — just a few nanometers, or billionths of a meter, thick — made of two *non*-superconducting cuprates (a metal and an insulator) actually exhibits superconductivity at the interface between the layers. This finding has triggered a debate about the super-property's origin and the possibility to turn the material's transition temperature thermostat higher.

But in order to reveal more information about this unique ultrathin film — which is made from a cuprate containing lanthanum, strontium, copper, and oxygen and appropriately called LSCO — scientists need a new set of tools that characterize the full film, not just the surface.

The researchers grew a variety of states of LSCO using a unique molecular beam epitaxy system at Brookhaven that allows materials to be deposited atom by atom, giving precise control of each layer's thickness. By varying the concentration of strontium in the cuprate, the scientists can create LSCO that behaves in three different ways: like a metal, an insulator, or a superconductor.

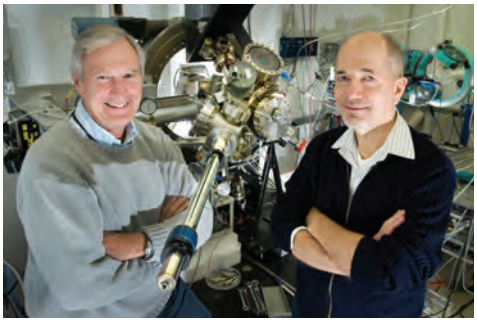
They then used x-ray diffraction at Argonne National Laboratory's Advanced Photon Source to determine the positions of the atoms inside the film. This was only possible by combining a synchrotron technique called coherent Bragg rod analysis (COBRA) with Difference Mapping, a slower but more accurate procedure. The result is a precise technique that's two orders of magnitude quicker than Difference Mapping alone.

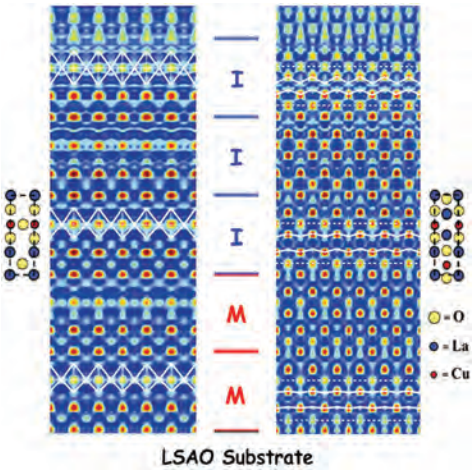
This diffraction data was used to map the distance of LSCO's out-of-plane (apical) oxygen atoms from the copper-oxygen plane, a characteristic known to affect the transition temperature of high-temperature superconductors.

The group's results showed an unexpected discrepancy. The apical distance stays the same in metallic and superconducting LSCO films but increases in the metallic-insulating LSCO bilayer films previously studied by the researchers.

These results show that the crystal structure of the few layers nearest to the surface can be very different from that inside the bulk — and in an unexpected ways.

H. Zhou, Y. Yacoby, V.Y. Butko, G. Logvenov, I. Božović, R. Pindak, "Anomalous Expansion of the Copper-Apical-Oxygen Distance in Superconducting Cuprate Bilayers," *PNAS*, **107**(18), 8103 (2010).





Left: Ron Pindak (left) and Ivan Božović at NSLS beamline X21, which could be upgraded to perform COBRA measurements as a jump-start program for NSLS-II.

Right: The measured electron density in two atomic planes of the interfacial superconducting bilayer LSCO film showing the positions of the atoms in two metallic (M) and three insulating (I) unit cells *Left:* in the (100) plane, the white lines highlight the projected shapes of the CuO_6 octahedra, in particular the elongation near the surface; *Right:* in (110) plane, the white lines highlight the projected profiles of the La-apical O planes, in particular the enhanced corrugation near the surface.

Key Difference in How TB Bacteria Degrade Doomed Proteins

Scientists at Brookhaven National Laboratory and Stony Brook University discovered a key difference in the way human cells and Mycobacterium tuberculosis bacteria, which cause TB, deliver unwanted proteins — marked with a "kiss of death" sequence — to their respective cellular recycling factories. This critical difference may help scientists design drugs to disable the bacterial system while leaving normal human protein recycling centers intact.

With tuberculosis infecting a third of the world's population, primarily in developing countries, there is great need for new, effective TB treatments. This research seeks to understand the protein-recycling mechanism of TB bacteria, because it is one of the microbe's keys to survival in human cells. Targeting this system with small-molecule-based drugs could inhibit the bacteria and effectively treat TB.

The catch is that human cells have a similar protein-recycling system, essential for their survival, which could also be destroyed by inhibitory drugs.

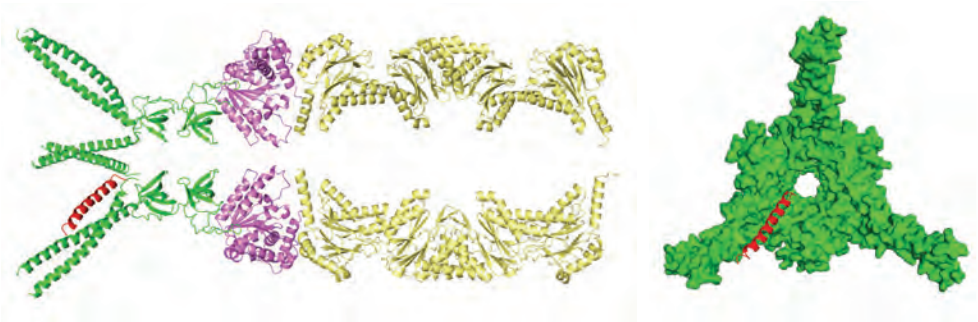
The researchers previously looked at differences in the cellular structure known as a proteasome that chops up the unwanted proteins. The current study examined the way proteins destined for degradation are recognized by the bacterial proteasome before entering that structure.

Using beams of high-intensity x-rays at NSLS beamlines X25 and X29, the scientists determined atomic-level structures of the portion of the bacterial proteasome that identifies the unwanted protein's "kiss of death" marker sequence — as well as structures of the marker sequence as it binds with the proteasome.

Based on the structures, the scientists describe a detailed mechanism by which coiled, tentacle-like arms protruding from the proteasome identify the death sentence label, causing a series of protein-folding maneuvers that pull the doomed protein into the degradation chamber.

Importantly, this interaction between the bacterial proteasome and the marker sequence is unique to bacteria. Human cells use a different marker protein and a completely different mechanism for drawing doomed proteins into the proteasome. Thus the details of proteasome-substrate interaction revealed by the current study may provide highly specific targets for the development of new anti-tuberculosis therapies.

T. Wang, K. Heran Darwin, and H. Li, "Binding-induced Folding of Prokaryotic Ubiquitin-like Protein on the Mycobacterium Proteasomal ATPase Targets Substrates for Degradation," *Nature Structural & Molecular Biology*, **17**, 1352 (2010).



Top left: Side view: These computer-generated images show how the "kiss of death" protein marker sequence (red) is recognized by and binds to one of three long tentacle-like structures of an enzyme (green) that sits at the entrance to the TB bacterium's protein-degradation chamber, or proteasome — shown to the right of the green region in the side view. The enzyme will unfold the marked protein and feed it into the proteasome for degradation.

Top right: Top view

Bottom: Brookhaven Lab researchers Huilin Li (standing) and Tao Wang

YEAR IN REVIEW

The NSLS-II construction site transformed from a field of dirt to a fully formed steel ring half a mile in circumference, a new education program introduced a different set of users – middle school and high school students – to invaluable experimental tools at NSLS, and three NSLS visiting scientists brought home a couple of the world's most prestigious scientific honors, the Nobel and Kavli prizes. Fiscal year 2010 was a busy year, to say the least. Here are highlights.

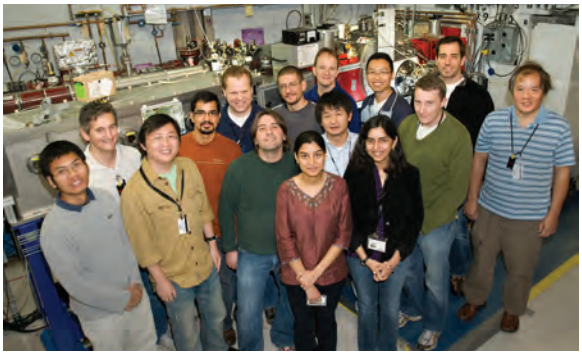
OCTOBER 2009

A Nobel for Atomic-level "Pictures" of Protein Factories

Two recipients of the 2009 Nobel Prize in Chemistry have strong ties to NSLS. Venki Ramakrishnan, a former employee in Brookhaven's biology department and long-time NSLS user, now at Cambridge University, and Thomas A. Steitz of Yale University, also a long-time NSLS user, shared the prize with Ada E. Yonath of the Weizmann Institute of Science for their work on the structure and function of the ribosome. In the late 1990s, Ramakrishnan and Steitz used protein crystallography at the NSLS and other light sources solve the high-resolution structures for two ribosome subunits crucial to understanding everything from how the ribosome achieves its amazing precision to how different antibiotics bind to it.

Contracts Awarded for Production of NSLS-II Storage Ring Magnets

The last of seven contracts for the production of the NSLS-II storage ring magnets are awarded. A total of 826 magnets will be built by vendors in China, Denmark, New Zealand, Russia, the United Kingdom, and the United States.



NSLS Hosts First Training Session on Solution X-ray Scattering

About a dozen researchers from eight different institutions gather at NSLS to learn the ways of solution x-ray scattering. The inaugural training session was based at X9, a newly commissioned beamline that specializes in taking small angle x-ray scattering measurements — data that are very valuable for studying biological macromolecules.

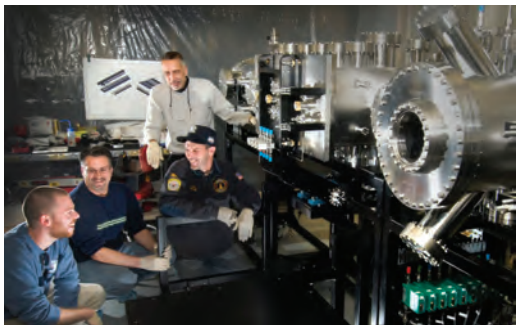
NOVEMBER 2009

Photo courtesy of The Kavli Prize

NSLS Users Take Home Prestigious Awards

Three NSLS users win a variety of honors. They include: New York University chemist Nadrian C. (Ned) Seeman (top left), who shared the 2010 Kavli Prize in Nanoscience for his pioneering advances in the field of DNA nanotechnology; Javier Pulecio (bottom middle), a doctoral student at the University of South Florida and a former NSLS summer intern who received the 2010 Hispanic Pathways Award in the student category; and National Institute of Standards and Technology scientist Joe Woicik (top right), who won a 2010 Department of Commerce Silver Medal for developing a novel, synchrotron-based x-ray spectroscopy method to accurately measure the site-specific nature of individual chemical bonds.

DECEMBER 2009



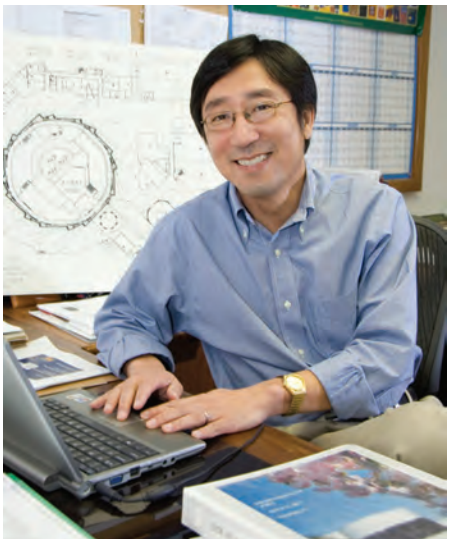
NSLS-II Project Unveils New Optics R&D Laboratory

A Brookhaven Lab building is renovated to provide general lab and clean room space dedicated to optics R&D. This new optics area provides cutting-edge capabilities in both reflective and transmission multilayer optics, crystal diffractive optics, surface metrology over a broad range of spatial resolutions, nanopositioning, and other nanofabrication required for NSLS-II.

Physicist Larry Carr Named APS Fellow

Larry Carr, a Photon Sciences physicist, is among six scientists at Brookhaven Lab to be named a Fellow of the American Physical Society. Carr was recognized for his applications of synchrotron and terahertz radiation to condensed-matter systems.

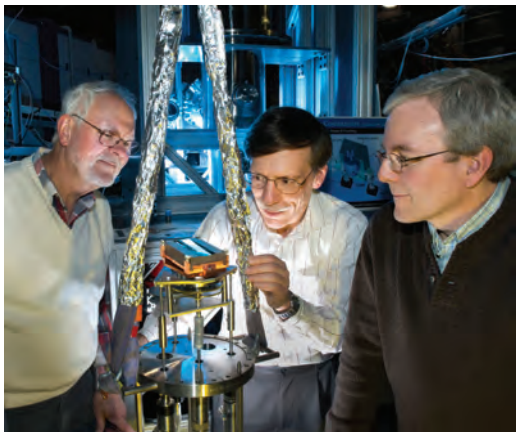
JANUARY 2010



Chi-Chang Kao Named AAAS Fellow

The American Association for the Advancement of Science awards NSLS Department Chair Chi-Chang Kao with the distinction of Fellow. Kao was recognized for "his many contributions to resonant elastic and inelastic x-ray scattering techniques and to x-ray spectroscopy, their applications to important materials, and his inspired leadership at the NSLS."

FEBRUARY 2010



Building NYS Business Opportunities

After learning that no U.S. companies are able to manufacture a particular type of synchrotron mirror, a group of researchers from Brookhaven, the National Institute of Standards and Technology, and R. Browning Consultants reaches out to a New-York-based company. The group worked with Optimax, which specializes in optics for cameras and telescopes, to produce the mirror for a new microscope at NSLS.

First Steel Arrives for NSLS-II Ring Building

The first shipment of steel beams dedicated for the NSLS-II ring building arrives at the construction site, starting the assembly of the interior skeleton of the ring building.

MARCH 2010

NYS Funds Collaborative Battery Research at NSLS

The New York State Energy Research and Development Authority awards $8 million in energy storage research grants, of which a little more than $3 million involve studies at NSLS. A $550,000 grant will fund a partnership between Brookhaven Lab, SUNY's University at Buffalo, and Binghamton University to develop improved batteries for use in stationary grid-scale energy storage applications. In addition, Brookhaven and Stony Brook University are teaming up with GE Global Research, which will receive $2.5 million to make improvements to its sodium metal halide batteries.

Scientist Ferdinand Willeke Granted Tenure

Photon Sciences Accelerator Division Director Ferdinand Willeke is granted tenure by Brookhaven Science Associates. Willeke was honored for his exceptional work on nonlinear beam dynamics; his contributions to the design, construction, operation and upgrade of the proton collider, HERA, of Deutsches Elektronen-Synchrotron (DESY) Laboratory in Germany; and his outstanding performance in directing the design and construction of the NSLS-II accelerator systems.

APRIL 2010

Scientists Get Funding to Design Anti-Botulism Drugs

Scientists at Brookhaven Lab, in collaboration with researchers at Stony Brook University, are selected to receive up to $1.4 million in applied research funds from the Department of Defense Threat Reduction Agency to develop drugs that block the paralytic and deadly effects of botulinum neurotoxins.

(c) 2009 ParnassusWorks. Photo by: Liza Politi

NSLS Featured in PBS Documentary

PBS affiliates across the country start airing a one-hour documentary on the trials and tribulations faced by aspiring scientists, filmed in part at NSLS. Recorded over three years, "Naturally Obsessed: The Making of a Scientist" follows a group of Columbia University student researchers as they study a protein that could reveal a new path toward the treatment of diabetes and obesity.

Take Our Children to Work Day Highlights the Wonders of Food

A group of nearly 50 children of Photon Sciences Directorate employees learn about the science — and fun — of food during national "Take our Daughters and Sons to Work Day." The crowd pleaser was a Mentos-soda experiment, which created a powerful and sticky geyser more than five feet tall.

MAY 2010

Climate Change, Clean Energy Define NSLS CFN Users' Meeting

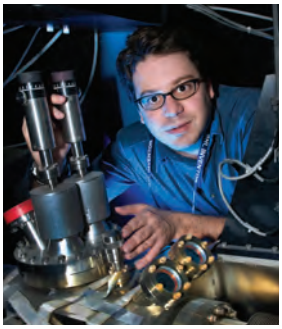
Highlighting the synergy between NSLS and Brookhaven's Center for Functional Nanomaterials, government, laboratory, and science leaders make an urgent call for the development of efficient and effective clean energy technologies at the annual meeting of the facilities' user communities. About 500 visiting scientists, staff members, and funding representatives gathered at Brookhaven for the joint meeting, which emphasized climate change and the tools scientists are using to combat it.

Bringing NSLS into the Classroom

A new program launched at Brookhaven lets high school teachers and their students conduct experiments they devise with a major piece of scientific equipment: NSLS. The program, dubbed In-SynC for Introducing Synchrotrons into the Classroom, allocates time on the multi-million-dollar machine to classrooms through a competitive, peer-reviewed proposal process.

Mike Caruso, Rick Greene Win UEC Community Service Awards

The NSLS Users' Executive Committee awards the 2010 UEC Community Service Award for outstanding service, innovation, and dedication to users of the NSLS to two recipients, Mike Caruso and Rick Greene. Caruso is a mechanical technician for the VUV beamlines and Greene is a mechanical technician for the x-ray beamlines.



2010 Baumert Award Goes to Jonathan Rameau

Jonathan Rameau, a post-doctoral researcher in Brookhaven's Condensed Matter Physics and Materials Science Department, receives the Julian Baumert Ph.D. Thesis Award for his work on high-temperature superconductors.

JUNE 2010

Light Sources Employees Honored with Prestigious BNL Awards

Five Light Sources Directorate employees are selected as recipients of Brookhaven's highest accolades. The awards, given to 15 BNLers lab wide, were received by Andrew Ackerman, Nathalie Bouet, Ray Conley, Thomas Nehring, and Charles Spataro.

New Tools for NSLS-II

The U.S. Department of Energy grants CD-0 (approval of mission need) for a Major Item of Equipment Project known as "NSLS-II Experimental Tools," or NEXT. The NEXT Project will design and construct 5-6 beamlines, and CD-0 authorized the start of their conceptual design.

Summer Student Invasion

More than 40 college students and professors arrive at Brookhaven to spend their summer at NSLS and NSLS-II. The students worked with staff in areas ranging from the study of Alzheimer's disease to the development of new software and instrumentation.

NSLS-II Call for Beamline Development Proposals Gets Huge Response

A remarkable 54 NSLS-II beamline development proposals are submitted by nearly 700 proposal team members from around the world. Each proposal was reviewed first by one of seven Science Advisory Committee (SAC) Study Panels and then by the full SAC. More than half — 34 — were approved.

JULY 2010

Hands-on Science Draws Record Crowd

Marshmallow Peeps, water rockets, liquid nitrogen, and a firsthand look at what will be one of the world's most advanced light sources attract a record-breaking number of visitors to NSLS and the NSLS-II construction site for a one-day open house. Nearly 1,190 people attended the event as part of Brookhaven Lab's Summer Sundays program.

Joint InSynC-INCREASE Meeting Brings Teachers, Professors to NSLS

More than 30 educators from two unique groups come to Brookhaven Lab to gain synchrotron skills for themselves and their students. Participants in the two groups — the Interdisciplinary Consortium for Research and Educational Access in Science and Engineering (INCREASE) and Introducing Synchrotrons into the Classroom (InSynC) — spent three days at NSLS to understand the basics of synchrotron mechanics, participate in hands-on demonstrations, and learn how to write a proposal for beam time.

AUGUST 2010

$34-Million Contract for Lab-Office Buildings

E.W. Howell, based in Plainview, NY, wins a $34-million contract to build laboratory-office buildings for NSLS-II. Construction is funded by the American Recovery and Reinvestment Act.

NSLS Chair Chi-Chang Kao Steps Down, Takes Lead at SSRL

Chi-Chang Kao, who served as chair of NSLS for four years, leaves Brookhaven to serve as Associate Laboratory Director for the Stanford Synchrotron Radiation Lightsource at SLAC National Accelerator Laboratory in California. Kao, who made breakthrough discoveries in fields ranging from optics to magnetism during his 22 years at NSLS, was replaced by Interim Chair Erik Johnson.

SEPTEMBER 2010

Moving Into Production for Accelerator Hardware

The Accelerator Division checks off 11 of its 14 goals for the year, with "in progress" noted on the balance. Design work on the complex hardware for NSLS-II accelerator systems was completed in 2010. This includes superconducting cavities, RF power sources, vacuum systems, power supplies, magnet systems and insertion devices. In addition, the division started the fabrication and assembly of aluminum vacuum chambers, finishing roughly 25 percent of them by year's end. Orders for all vacuum pumps were placed, and about 50 percent of the pumps were delivered.

Designing the First NSLS-II Beamlines

Preliminary designs are completed for the first six NSLS-II project beamlines. The designs lay out basic beamline details, from the front ends, where the light is siphoned off the main ring, to the hutches, where research is performed.

Closing the Ring

The structural framework of NSLS-II becomes a complete, nearly half-mile ring as the final steel beam is bolted into place. The "topping out" ceremony collected the signatures of more than 300 construction workers, Brookhaven and Department of Energy officials, invited guests, and Lab employees on the last steel beam, which will be visible to future research teams on the experimental floor.

Boom Gives Birth to Photon Sciences Directorate

The Light Sources Directorate spends much of the year planning for a reorganization into the Photon Sciences Directorate. This new structure will better manage the rapid growth of the directorate, which grew from 180 employees to 450 in five years as its portfolio expanded from operating NSLS to also include designing and constructing NSLS-II, designing and constructing additional beamlines for NSLS-II and, in coming years, transitioning to NSLS-II operations.

FACILITIES

"We are ahead of schedule and within budget on construction of the basic buildings and utilities for NSLS-II. Teamwork is key to our success."

- Martin Fallier
Director, Facilities Division

The Quick Pace of Construction

Compare the pictures taken October 2009 and September 2010 (below). They show the remarkable progress made this year on NSLS-II construction, evidence of the hard work of everyone involved — from Photon Sciences staff to construction workers on the site.

The Facilities Division, responsible for the design and construction of conventional facilities within the Photon Sciences Directorate, is necessarily focused on NSLS-II. With a budget of $912 million and an official completion date of 2015, NSLS-II is the largest domestic capital project under construction by the Department of Energy's Office of Science.

Construction of the facility is expected to create more than 1,250 construction jobs and 450 scientific, engineering, and support jobs, plus additional jobs at U.S. material suppliers and service providers. By the time conventional construction is complete, Brookhaven Lab will have purchased $120 million in labor and $115 million in materials for the basic buildings and utilities.

For fiscal year 2010, the division concentrated on the following:

- constructing the ring building, which will house the accelerator and the experimental facilities
- expanding the Laboratory's utility infrastructure, which includes adding 2,500 tons of cooling capacity to the existing chilled water plant and 20 megavolt amperes capacity to the Lab's main electrical substation for the added requirements of NSLS-II
- issuing the contract for laboratory-office buildings (LOBs)

Because of the accelerator tunnel and the robust construction of the ring building, concrete placement was the critical path for much of the year. Unseasonably cold weather and major snowfall events during the winter season led to a frost depth of nearly 15 inches. Despite the challenging weather, overall progress continued to be on or ahead of schedule, as the general contractor, Torcon, was able to finish key activities on the critical path. For example, Torcon placed a record 3,854 cubic yards of concrete in April 2010 — 1,727 cubic yards more than what was planned for that month.

The LOB contract was awarded in August 2010 to E.W. Howell, following months of work to finalize the design and complete the procurement process. Funding for the LOBs comes from the American Recovery and Reinvestment Act (ARRA). The NSLS-II Project received $150 million in ARRA funding, $34 million of which was designated for the LOBs.

At year's end, the NSLS-II Project was 37 percent complete, and the division looked forward to a "topping out" celebration. In the construction industry, workers sign the last steel beam before it's bolted into place, completing the structural steel framework of a building. That construction milestone was just around the corner.

Top: NSLS-II construction site, October 2009

Bottom: NSLS-II construction site, September 2010

About the Facilities

NSLS

- Began operating in 1982
- FY10 operating budget of $38.5 million
- Over 2,000 scientists come each year to do experiments
- 60 beamlines: 49 on X-Ray Ring and 11 on Vacuum Ultraviolet Ring
- VUV Ring operating energy: 800 MeV
- X-Ray Ring operating energy: 2.8 GeV
- Runs 24 hours a day, seven days a week, more than 250 days a year
- Injection system accelerates electrons to 99.99998 percent light speed

NSLS-II

- Will be 10,000 times brighter than NSLS, with 3 GeV ring energy and 500 mA stored current with top-off injection
- At full capacity, will have more than 60 beamlines
- Construction requires 2,900 tons of steel and 41,000 cubic yards of concrete
- Will have 600,000 square feet of space total
- Ring building, nearing completion, has outside circumference of 913 meters (just over half a mile)
- When operating, will draw up to 20 megawatts of power
- Will require 2,500 tons of mechanical refrigeration and 1,800 tons of cooling tower capacity

NSLS-II Digs up History

Five years before becoming fully operational, NSLS-II already is leading to discoveries – of the historical kind. As earthwork takes place on the NSLS-II construction site, which housed part of Camp Upton in the World War I and II era, artifacts ranging from rusted horseshoes to nearly 100-year-old pieces of newspaper are being dug up.

The most recent find is a large piece of painted concrete rock thought to have been part of a floor in a warehouse used in the army base in the 1940s. The rock, which has a hand-drawn emblem of a bugle, the notation "Company G" and the logo "Baptized by Fire," was identified with the 14th regiment, known as the "Fighting Fourteenth" and the "Red-legged Devils" from Brooklyn.

Construction workers also recently discovered a WWII dog tag that belonged to a solider who likely passed through Camp Upton on his way to England.

These artifacts are a few of many. In fact, a makeshift museum of Sheffield milk bottles, railroad spikes, Coca-Cola glasses — even a delicately etched Ed. Pinaud hair tonic bottle — has been made out of a table in the NSLS-II Project construction trailer, where passersby can imagine what life was like in Upton nearly a century ago.

Left: The inscribed concrete boulder found on the NSLS-II excavation site

Right: The dig find "museum" in the NSLS-II Project construction trailer

1

2

3

4

5

NSLS-II Construction Milestones

November 2008
Site prep work begins for ring building

January 2009
DOE approves construction start

February 2009
Torcon selected as general contractor for ring building

February 2009
New York State announces allocation of low-cost electricity to support construction

March 2009
DOE allocates $184.3 million from Recovery Act to Brookhaven Lab, principally to accelerate construction

June 2009
Formal groundbreaking ceremony to mark construction start *(Photo 1)*

July 2009
First concrete poured for ring building (*Photo 2)*

September 2009
First eight pieces of structural steel installed as part of utility and vehicle tunnels under ring building *(Photo 3)*

October 2009
Cut and fill operations for ring building ends, ensuring stable foundation

November 2009
First high-density concrete poured for shielding

December 2009
Proposals solicited for design package for lab-office buildings

February 2010
First structural steel erected for aboveground portion of ring building; continuous steel erection begins

March 2010
First steel arrives for ring building *(Photo 4)*

August 2010
E.W. Howell selected as general contractor for lab-office buildings attached to ring building *(Photo 5)*

ACCELERATOR

"We had 14 goals for the year and checked off 11, with 'in progress' noted on the balance. This achievement is a testament to the talent and hard work of the Accelerator Division staff, our vendors, and our supporters at Brookhaven and elsewhere."

- Ferdinand Willeke
Director, Accelerator Division

Accelerator Division Delivers Reliable NSLS Beams, Key NSLS-II Components

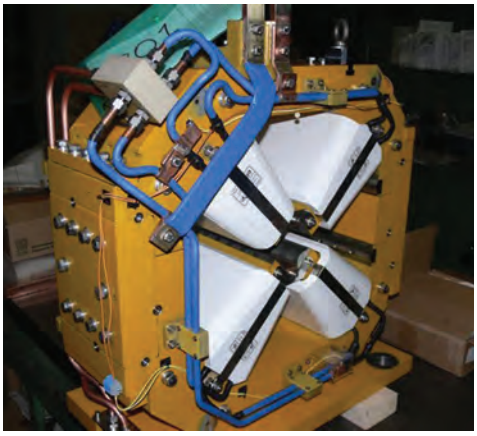
The Photon Sciences Accelerator Division had a full workload in 2010. While it was generally business as usual at NSLS, maintaining an older synchrotron at a high performance level is not easy. The NSLS-II Project placed increasing demands on the division, with 2010 seeing great growth in construction and design, and preparations ongoing for the eventual transition from NSLS to the new facility.

NSLS has been operating for more than 30 years, but Accelerator Division staff members are still finding ways to keep it running reliably, despite the extensive preventative maintenance the facility needs. This year, the division's efforts at NSLS involved aggressively maintaining the aged hardware system, replacing systems when necessary, providing spares for critical systems, and coming up with alternative solutions when replacing hardware didn't make sense considering the relatively short time until NSLS stops running.

Among the many regular tasks involved are polishing exposed high-voltage parts, inspecting power supplies and electronics, cleaning heat exchangers and filters, and replacing fans and other parts that tend to wear out quickly. On the X-ray Ring, activities continued for the ongoing upgrade of the radio-frequency power source. And in early 2010 the division completed a major job: the removal of a corroded water-cooling tower on the NSLS roof and the installation of a new one.

At NSLS-II, the Accelerator Division oversaw several production milestones. There was a great deal of progress in magnet production, beginning in February with a delivery of the first completed sextupole magnet. Several other "first article" magnets later arrived and staff began testing them for proper magnetic field quality and other key specifications. Magnet production and delivery was generally slower than expected, however, due to some initial manufacturing issues experienced by vendors.

The division awarded contracts for the NSLS-II linear accelerator and booster ring, and reviewed design and production schedules for both machines. There was also great progress in the production of girders, vacuum systems, power supplies, and electronic components. Staff began designing NSLS-II's many insertion devices and awarded a contract for the damping wiggler. They also awarded most of the contracts for the power supply components.



NSLS-II storage ring magnets — a total of 826 — include quadrupoles **(left)** and dipoles **(right)**. The magnets are being built by vendors in six countries: China, Denmark, New Zealand, Russia, the United Kingdom, and the United States.

NSLS-II's Beam Position Monitoring System

One of the many built-in technologies that will make NSLS-II one of the most advanced synchrotrons in the world is the system that will monitor the position of the electron beam as it circles the main ring.

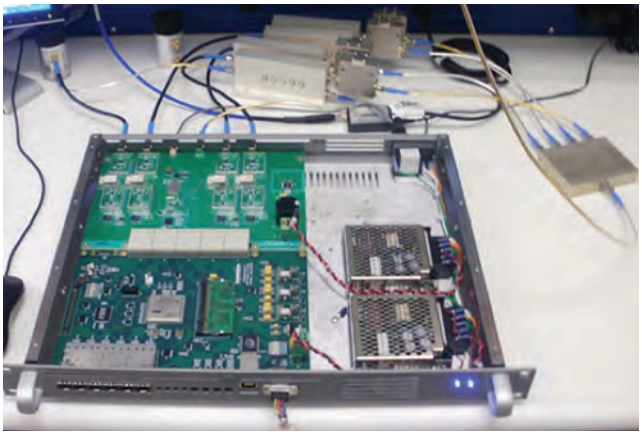
To deliver light of the highest quality, the beam must be ultra-stable: It cannot stray more than 200 nanometers in the vertical direction. This level of stability is unprecedented and, accordingly, requires a highly advanced beam position monitoring (BPM) system.

The mechanical requirements for the system's diagnostics and instrumentation are extremely challenging. Research and development of the BPM began in August 2009 and made significant progress in fiscal year 2010. The system will consist, in part, of more than 300 individual monitors – 60 in the injection system and approximately 250 placed around the main storage ring. The monitors will each have two circular electrodes, known as "button pick-ups," that will detect position-dependent electrical impulses from the beam. This information is then converted to digital data and distributed to computers in the NSLS-II control room to be analyzed and displayed. It takes only one 10,000th of a second for a complete set of beam-orbit data to be collected, which allows even the tiniest deviation of the beam orbit to be corrected. It is in this way that the extreme orbit stability of NSLS-II is maintained.

As they design the system, the NSLS-II diagnostics team is very concerned how thermal effects will impact the long-term performance of the BPM. Powerful microwaves generated in the beam vacuum chamber can substantially heat certain BPM components, such as the button pick-ups, causing them to expand and the monitor to malfunction. The team must come up with solutions to these issues. For example, they decided to make the buttons from molybdenum, a metal with high electrical and thermal conductivity.

The first test of the system took place in June at the Advanced Light Source in Berkeley, California, and was successful. The test also showed that the system as it is currently designed will hold up well over time.

Beam position monitoring system



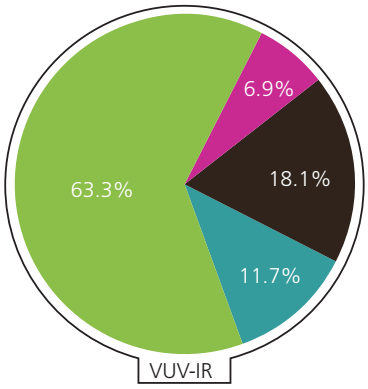
NSLS reliability

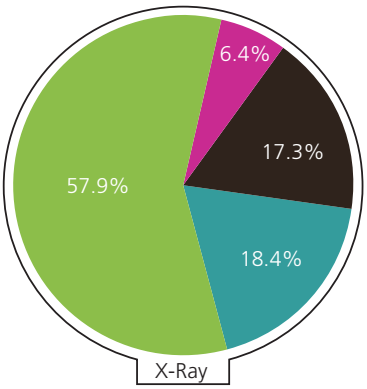
The NSLS served up another excellent year, with the X-Ray Ring coming in at 95.4 percent reliability and 109.1 percent availability. The VUV Ring performed even better, at 98.2 percent and 110.1 percent, respectively. Both reliability, the ratio of delivered beam time to scheduled beam time, and availability, which is very similar but also accounts for available beam time that wasn't originally scheduled, are a measure of the machine's performance. Such high percentages, all the more impressive considering the age of the facility and a tight budget, are a testament to a stellar staff.

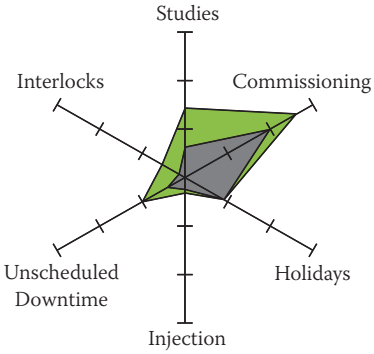
X-Ray and VUV-IR Parameters

	X-Ray	VUV-IR
Energy	2.800 GeV	0.808 GeV
Maximum Current	300 mA	1.0 A
Photon Critical Wavelength (Energy) for Dipole	1.75 Å (7.1 keV)	20.3 Å (612 eV)
Photon Critical Wavelength (Energy) for X17 wiggler at 4.2T	0.57 Å (22 keV)	
Horizontal Emittance	62 nm-rad	160 nm-rad
Vertical Emittance	0.34 nm-rad	≥ 0.35 nm-rad (4 nm-rad in normal ops.)
Electron Orbital Period	567.2 nanoseconds	170.2 nanoseconds
Number of RF Buckets	30	9
Typical Bunch Mode	30	7
Natural RMS Energy Spread	9.2×10^{-4}	5.0×10^{-4} ($I_b < 20$ mA)
RMS Bunch Length	44 mm	5 cm ($I_b < 20$ mA)

FY2010 NSLS Machine Activities





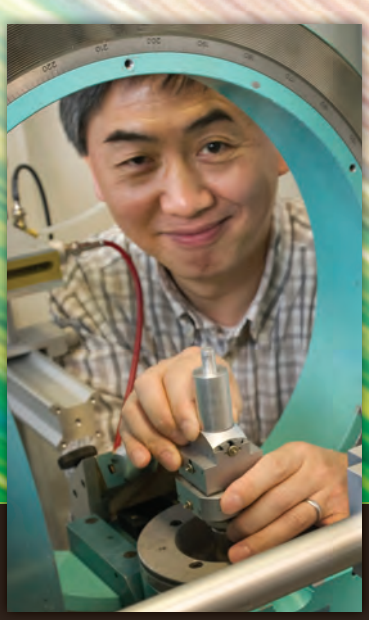


- Scheduled Operations
- Unscheduled Operations
- Maintenance
- Other - Studies, Com/Con, Holiday, Injection, Unscheduled downtime, Interlock

Other Activities	VUV/IR	X-Ray
Studies	1.7%	3.8%
Com/Con	5.4%	7.0%
Holiday	2.5%	2.5%
Injection	0.7%	0.9%
Unsched. downtime	1.1%	2.7%
Interlock	0.4%	1.5%

User Metrics	VUV/IR	X-Ray
Reliability	98.2%	95.4%
Availability	109.0%	106.0%

BEAMLINES



"Synchrotron sources have quickly become an essential tool for a wide spectrum of research. All the action takes place at beamlines, each one consisting of a suite of sophisticated scientific instruments. The robust beamlines at NSLS produce remarkable science, and we made excellent progress on developing NSLS-II beamlines and associated science programs."

- Qun Shen
Director, Photon Division

Beamline & Optics R&D: Enhancing Tools at NSLS, NSLS-II

While keeping the existing ring and beamline mechanical systems running, Photon Sciences staff completed a number of R&D projects this year that will enhance the tools of researchers at NSLS and, in the near future, NSLS-II.

One of the major accomplishments was the installation and commissioning of NSLS beamline X17A, which is optimized for x-ray total scattering and atomic pair distribution function (PDF) experiments. The new beamline will alleviate the large demand for beam time on high-energy beamlines X17B1, X17B2, and X17B3. The scientific focus of X17A will be the structural characterization of disordered, nanocrystalline and complex nanostructured bulk materials at ambient and extreme conditions. The beamline features a novel Laue diffraction monochromator design that uses two-axis bending of the silicon crystal to simultaneously focus the beam in two orthogonal planes. Due to the bending, lattice strain increases integrated reflectivity of the Laue diffraction crystal by an order of magnitude compared to a perfect crystal. Anticlastic bending, a natural phenomenon for a crystal under strain, is typically considered a nuisance that must be "controlled." In this case, it allows meridional focusing. A bender design, one that holds a rectangular crystal at the corners and bends it at the edges, makes slight adjustments to the "natural" anticlastic curvature to give the two-dimensional focusing.

Also this year, researchers developed a new method for measuring x-ray optics aberrations. Creating the very small x-ray spots used for

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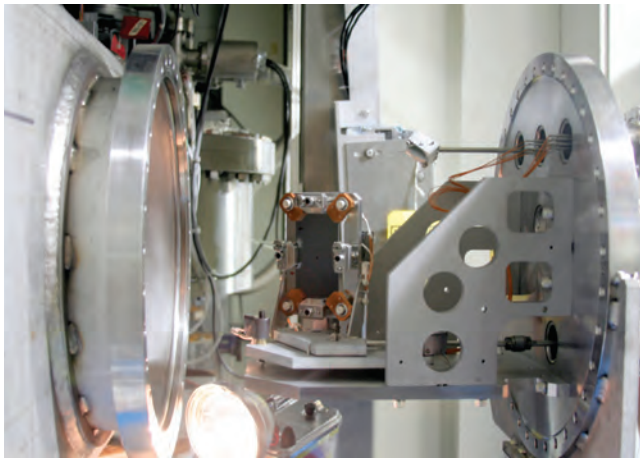

The X17A monochromator in the X17 front end, shown when rolled out of the chamber

Lens Development for X-ray Nanofocusing at NSLS-II

NSLS-II will use a wedged multilayer Laue lens (MLL) to achieve an unprecedented level of x-ray nanofocusing. MLLs are fabricated by magnetron sputter deposition onto small silicon blanks. They consist of many thousands of layers, with a total growth thickness goal of about 100 microns.

In 2009, the optics R&D lab designed and built a new magnetron sputtering system in collaboration with CVD Equipment Corporation in Ronkonkoma, NY. The system consists of a 23-foot, ultra-high vacuum chamber containing nine magnetron-sputtering guns, four cryogenic pumps, and a high-precision, linear-motion platform to enable the guns to deposit a stack of multi-film layers. The latest growths have been 43 microns thick with 6,510 layers and grew continuously for five days. All three metrics are records.

Multilayer Laue lens (MLL) deposition system, built in collaboration with CVD Equipment Corporation in Ronkonkoma, NY.

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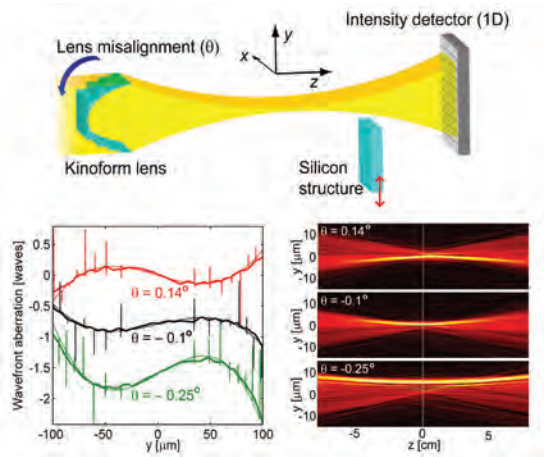
synchrotron nanoscale research requires a specialized and nearly perfectly formed optic to modify the phase profile of the beam. To look for aberrations — errors in the phase profile due to the optics (which can broaden and distort the spots) — scientists usually scan a slab of metal called a knife edge across the beam face. But to measure the beam size accurately with this method, the knife edge must be smaller than the beam. This is a problem for the types of nanoscience experiments planned at NSLS-II, where the beam is so small that the knife edge would have to be just one atomic plane thick — much too thin to fabricate. Photon Sciences researchers, along with colleagues at Argonne National Laboratory, the University of Rochester, and Cornell University, have figured out how to use an alternative called phase retrieval. The technique allows researchers to scan the beam with much larger feature sizes and then mathematically reconstruct the data to characterize the beam and its aberrations at any point along its path.

Other achievements made in 2010 were the installation of a transmission x-ray microscope at beamline X8C and the use of a wedged multilayer Laue lens to reach a record level of x-ray nanofocusing (see sidebars), and the creation of a large scanning stage that allows researchers to take x-ray fluorescence images of hefty items like paintings in a very short time frame. Art historians have been particularly interested in the latter development as a way to test the authenticity and genesis of artwork.



Top: Experimental setup of the phase retrieval technique. Bottom: Measured and simulated lens aberrations (left) and their corresponding through-focus amplitude of reconstructions (right) for different lens angular misalignments. (From Manuel Guizar-Sicairos et al., *Appl. Phys. Lett.* **98**, 111108 [2011])

New NSLS Transmission X-ray Microscope Enhances Nanoscale Studies

A new microscope installed this year will give NSLS users a powerful way to image energy storage materials, microelectronics, and biofuels. The transmission x-ray microscope (TXM), mounted at beamline X8C for use with hard x-rays, has an application energy range of 5,000-11,000 electron volts, and a target imaging resolution of 30 nanometers.

NSLS was awarded $2 million in American Recovery and Reinvestment Act (ARRA) funding to purchase the microscope — called the nanoXCT-S200. It was ordered from Xradia, Inc., headquartered in California, and will play an important role in the future of photon science research at Brookhaven Lab. With future funding anticipated, the microscope will be moved to a superconducting wiggler source at NSLS-II.

Left: Transmission x-ray microscope

Right: Brookhaven scientist Jun Wang at beamline X8C

Project Beamlines

Much of the year was spent on design work for the six project beamlines, with each completing a preliminary design report (PDR) in September 2010. The completed designs include engineering details sufficiently mature to begin long-lead-time procurements of major beamline systems, such as radiation enclosures and optical systems. Motion controllers are being tested and specifications are being written for a standard unit.

The **coherent hard x-ray scattering (CHX)** beamline design is complete, with a carefully optimized optics layout that will ensure that the beam stability required for the experiments will be achieved. The endstation design, including the SAXS and WAXS instruments, is complete.

The **coherent soft x-ray scattering/polarization (CSX)** beamline optical design was completed and the beamline was ready for purchasing the major optical components. The specifications for the elliptically polarized undulators were approved with the insertion device group, and advances were made working with the accelerator group to finalize the design of the straight section.

The **hard x-ray nanoprobe (HXN)** team continued to develop nanopositioning techniques. Testing of piezo scanning stages and laser interferometers in the lab yielded encouraging results, and a preliminary design of an MLL microscope is in progress.

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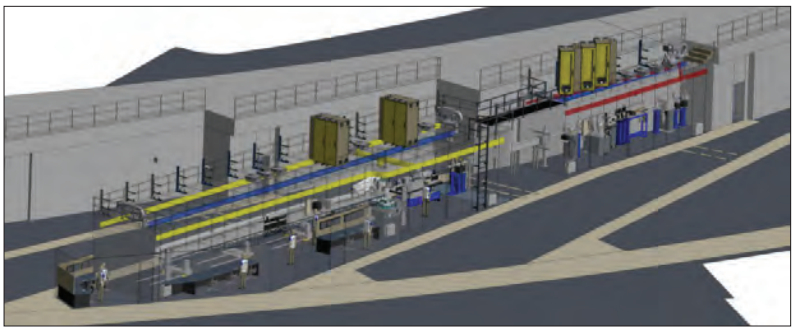

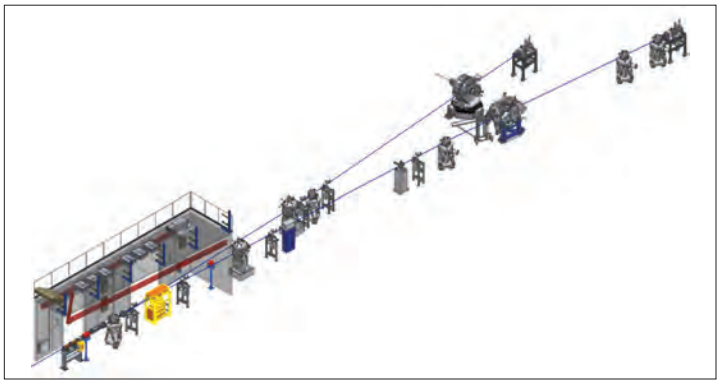

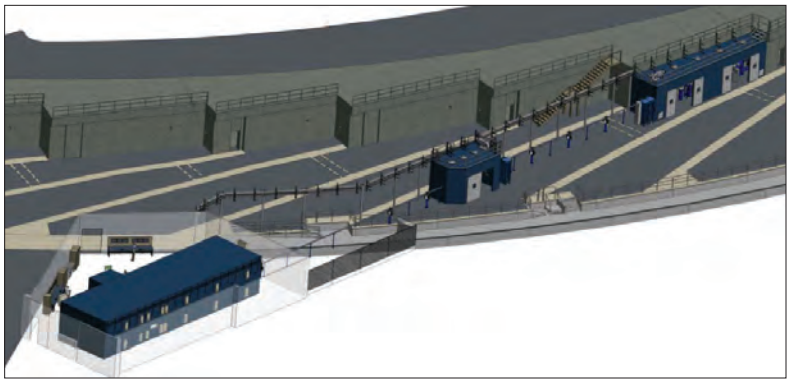

Beamline layouts from PDRs, September 2010.

Top: Coherent hard x-ray scattering

Middle: Coherent soft x-ray scattering/polarization

Bottom: Hard x-ray nanoprobe

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The **inelastic x-ray scattering (IXS)** team completed the mirror upgrade of the R&D beamline at NSLS, improving brightness by 10 times. Together with improvement in crystal quality, the resolution function of the CDW-CDW test carried out on the beamline achieved extremely sharp tails, reaching a critical milestone. Optical metrology and x-ray tests of the multilayer Montel mirror were completed and showed expected performance.

The **sub-mm resolution x-ray spectroscopy (SRX)** beamline is an in-vacuum undulator beamline that uses K-B mirrors for focusing. It is designed to eventually accomodate a second in-vacuum undulator beamline canted by 2-milliradians and using zone plates for focusing. The K-B beamline design is complete and the endstation design is progressing.

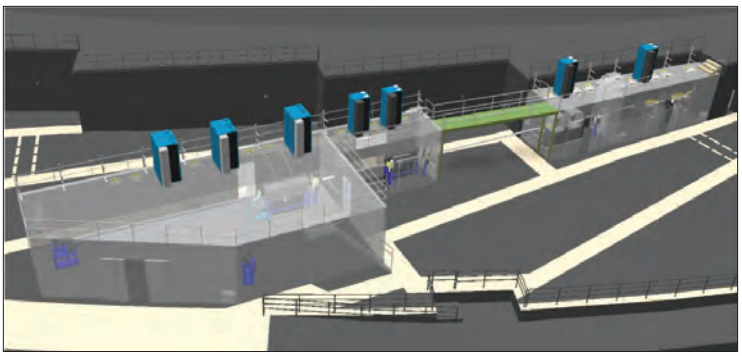
The optical layout of the two-branches of the **x-ray powder diffraction (XPD)** beamline was modeled and optimized to achieve the best possible flux throughput, tailored to the high energy, large divergence beam delivered by the damping wiggler source. For enhanced performance, the optics includes a novel sagittally bent double Laue crystal monochromator similar in concept to the NSLS monochromators in operation at beamlines X17B and X7B. Special attention was devoted to the high power and high heat load management.

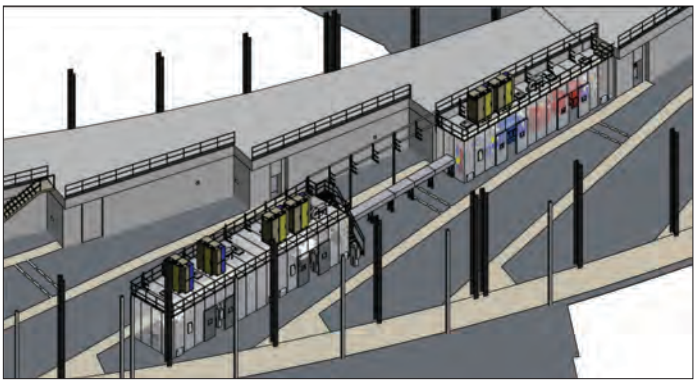
Beamline layouts from PDRs, September 2010.

Top: Inelastic x-ray scattering

Middle: Sub-mm resolution x-ray spectroscopy

Bottom: X-ray powder diffraction





Detector R&D

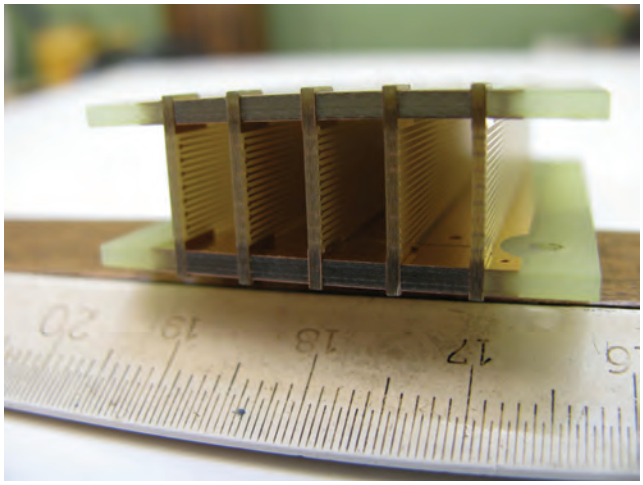
Detectors sit at the very end of the intricate systems that constitute light sources like NSLS and NSLS-II. Because detectors are where the science gets done, detector research and development can enable new science.

For the user community, NSLS-II will offer a significantly higher degree of coherence in its beams than most other synchrotrons, so imaging techniques that take advantage of that superiority are at the forefront of detector R&D.

The CHX beamline, one of six project beamlines being built for NSLS-II, uses photon correlation spectroscopy. The goal is to detect the arrival time of photons with the highest possible resolution over the largest possible area. Current detectors allow a time resolution in the millisecond range and require the full detector area to be read out with millisecond frame rate. The detector being developed will provide a time resolution of 10 microseconds in the first generation and around 10 nanoseconds in the next. DOE is funding this effort, which is a collaboration involving Brookhaven, Fermilab, and AGH University of Science and Technology in Poland.

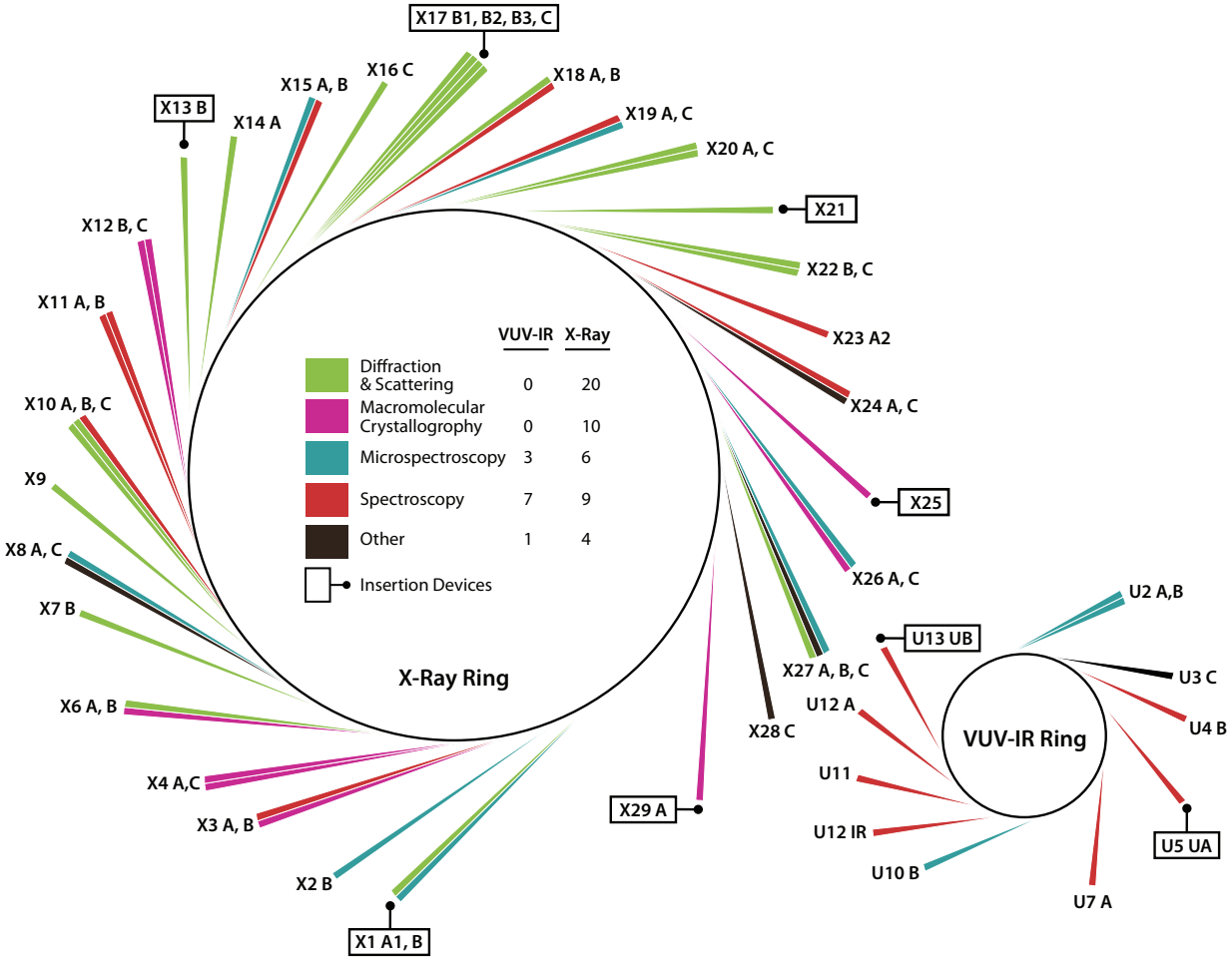
Another project beamline at NSLS-II, XPD, will enable diffraction using x-rays in the 50-100 keV range. At these energies, silicon becomes very transparent, so any silicon-based detector will be extremely inefficient. Work has begun on a technology based on germanium, which is much more highly absorbing in this energy range. Although this is extremely challenging, success will enable a range of new detectors and a new generation of experiments making use of high-energy x-rays.

Detector R&D can also help NSLS users to do better experiments. One user from the National Institute of Standards and Technology presented a challenge: Measure samples simultaneously using a technique known as EXAFS. The solution: A miniature four-channel ionization chamber was developed, providing an excellent way to do comparative experiments. A bonus: These devices have also proved useful at the Advanced Photon Source at Argonne National Laboratory.



A miniature four-channel ionization chamber that was developed at NSLS

Beamline Status



FY10 Beamline Guide

In 2010, 49 X-Ray and 11 Vacuum Ultraviolet-Infrared operational beamlines were available for a wide range of experiments using a variety of techniques.

There are two types of beamlines at NSLS: facility beamlines, of which there were 21; and participating research team (PRT) beamlines, of which there were 39. Facility beamlines are operated by Photon Sciences staff members and reserve a minimum of 50 percent of their beam time for general users. PRT beamlines are run by user groups with similar interests and reserve 25 percent of their beam time for general users, although they can grant additional time at their own discretion.

The following pages provide details on NSLS operational beamlines, including their unique characteristics.

Beamline Guide Abbreviations

ARPES	Photoelectron Spectroscopy, Angle-Resolved	**PRT**	Participating Research Team
DAFS	X-Ray Diffraction Anomalous Fine Structure	**SAXS**	Small Angle X-Ray Scattering
DEI	Diffraction-Enhanced Imaging	**STXM**	Scanning Transmission X-Ray Microscopy
EXAFS	X-Ray Absorption Spectroscopy, Extended Fine Structure	**UPS**	UV Photoelectron Spectroscopy
FB	Facility Beamline	**UV-CD**	Ultraviolet Circular Dichroism
HARMST	High Aspect Ratio Microsystems Technology	**WAXD**	Wide-Angle X-Ray Diffraction
IRMS	Infrared Microspectroscopy	**WAXS**	Wide-Angle X-Ray Scattering
MAD	Multi-Wavelength Anomalous Dispersion	**XAS**	X-Ray Absorption Spectroscopy
MCD	Magnetic Circular Dichroism	**XPS**	X-Ray Photoelectron Spectroscopy
NEXAFS	Near Edge X-Ray Absorption Spectroscopy	**XRD**	X-Ray Diffraction
PEEM	Photo Emission Electron Microscopy		

Beamline	Source	Type of Research	Energy Range	Type	Organization
VUV-IR Beamlines					
U2A	Bend	IRMS High pressure research IR spectroscopy	30-10000cm-1	FB	BNL-NSLS Carnegie Institution of Washington COMPRES
U2B	Bend	InSynC - Education IRMS	500-4000 cm-1	FB	BNL-NSLS
U3C	Bend	Metrology	50-1000 eV	PRT	Lawrence Livermore National Laboratory Los Alamos National Laboratory National Security Technologies Sandia National Laboratories
U4B	Bend	X-ray reflectivity X-ray scattering, magnetic X-ray scattering, resonant MCD XAS X-ray fluorescence spectroscopy	20-1200 eV	FB	BNL-NSLS Montana State University
U5UA	Insertion Device	ARPES UPS, spin-resolved	15-150 eV	FB	BNL-NSLS BNL-CFN
U7A	Bend	NEXAFS XPS	180-1200 eV	PRT	BNL-Chemistry Dow Chemical Company National Institute of Standards & Technology
U10B	Bend	IRMS	500-4000 cm-1	FB	BNL-NSLS
U11	Bend	UV-CD	3-10 eV	PRT	BNL-Biology
U12A	Bend	XAS XPS	100-800 eV	PRT	Oak Ridge National Laboratory
U12IR	Bend	IR spectroscopy Magnetospectroscopy THz / millimeter wave spectroscopy Time-resolved spectroscopy	8-20000 cm-1	FB	BNL-NSLS
U13UB	Insertion Device	UPS ARPES	3-30 eV	PRT	Boston University BNL-Physics Columbia University

Beamline	Source	Type of Research	Energy Range	Type	Organization
X-Ray Beamlines					
X1A1	Insertion Device	STXM NEXAFS	0.25-0.50 keV	PRT	BNL-CFN BNL-CMPMS SUNY @ Plattsburgh
X1B	Insertion Device	XAS X-ray fluorescence spectroscopy XPS	0.2-1.6 keV	PRT	Boston University Thomas Jefferson National Accelerator Facility University of Illinois
X2B	Bend	X-ray microtomography	8-35 keV	PRT	ExxonMobil Research and Engineering Co.
X3A	Bend	MAD Macromolecular crystallography	4.6-15.1 keV	PRT	Case Western Reserve University Rockefeller University Sloan-Kettering Institute for Cancer Research
X3B	Bend	XAS EXAFS	3.8-13.3 keV	PRT	Case Western Reserve University
X4A	Bend	MAD Macromolecular crystallography	3.5-20 keV	PRT	Albert Einstein College of Medicine City University of New York (CUNY) Columbia University Cornell University Mount Sinai School of Medicine New York Structural Biology Center New York University SUNY @ Buffalo Sloan-Kettering Institute for Cancer Research Wadsworth Center
X4C	Bend	MAD Macromolecular crystallography	7-20 keV	PRT	Albert Einstein College of Medicine City University of New York (CUNY) Columbia University Cornell University Mount Sinai School of Medicine New York Structural Biology Center New York University Rockefeller University SUNY @ Buffalo Sloan-Kettering Institute for Cancer Research Wadsworth Center
X6A	Bend	MAD Macromolecular crystallography	6-23 keV	FB	BNL-NSLS
X6B	Bend	XRD, surface WAXD X-ray reflectivity	6.5-19 keV	FB	BNL-NSLS
X7B	Bend	XRD, single crystal XRD, time resolved WAXD WAXS	25-50 keV	PRT	BNL-Chemistry General Electric
X8A	Bend	Metrology	1.0-5.9 keV	PRT	Lawrence Livermore National Laboratory Los Alamos National Laboratory National Security Technologies Sandia National Laboratories
X8C	Bend	MAD Macromolecular crystallography	5-19 keV	PRT	Biogen Incorporated Biotechnology Research Institute Hoffmann-La Roche National Institutes of Health
X9	Bend	X-ray Scattering, biomolecular solution SAXS WAXS	2.1-20 keV	FB	BNL-NSLS BNL-CFN

Beamline	Source	Type of Research	Energy Range	Type	Organization
X10A	Bend	XRD, powder WAXD SAXS WAXS	8-11 keV	PRT	ExxonMobil Research and Engineering Co.
X10B	Bend	XRD, powder XRD, surface WAXD X-ray reflectivity X-ray scattering, surface WAXS	14 keV	PRT	ExxonMobil Research and Engineering Co.
X10C	Bend	XAS EXAFS NEXAFS	4-24 keV	PRT	ExxonMobil Research and Engineering Co.
X11A	Bend	DAFS XAS EXAFS NEXAFS	4.5-40 keV	PRT	BNL-Material Sciences BNL-Environmental Sciences Canadian Light Source ETH Labs - Zuerich Natural Resources Canada Naval Research Laboratory (NRL) Naval Surface Warfare Center New Jersey Institute of Technology North Carolina State University Sarah Lawrence College Stony Brook University
X11B	Bend	XAS EXAFS NEXAFS	5-23 keV	PRT	BNL-Environmental Sciences BNL-Material Sciences Canadian Light Source ETH Labs - Zuerich Natural Resources Canada Naval Research Laboratory (NRL) Naval Surface Warfare Center New Jersey Institute of Technology North Carolina State University Sarah Lawrence College Stony Brook University
X12B	Bend	MAD Macromolecular crystallography	5-20 keV	PRT	BNL-Biology
X12C	Bend	MAD Macromolecular crystallography	5.5-20.0 keV	PRT	BNL-Biology
X13B	Insertion Device	Microdiffraction Imaging	9-16 keV	FB	BNL-NSLS Columbia University
X14A	Bend	MAD XRD, powder XRD, single crystal XRD, time resolved WAXD X-ray reflectivity	6-22 keV	PRT	New Jersey Institute of Technology New York State College of Ceramics Oak Ridge National Laboratory University of Tennessee
X15A	Bend	DEI	10-60 keV	FB	BNL-NSLS
X15B	Bend	XAS EXAFS NEXAFS	0.8-15 keV	PRT	Corning, Inc. Georgia Institute of Technology Lawrence Berkeley National Laboratory Lucent Technologies, Inc. Miami University North Carolina State University Princeton University Stony Brook University University of Delaware Woods Hole Oceanographic Institute

Beamline	Source	Type of Research	Energy Range	Type	Organization
X16C	Bend	XRD, powder	6.5-25 keV	PRT	Stony Brook University
X17B1	Insertion Device	XRD, powder	20-150 keV	FB	BNL-NSLS Rutgers University
X17B2	Insertion Device	XRD, powder XRD, time resolved High pressure research	20-130 keV	FB	BNL-NSLS COMPRES Stony Brook University - Mineral Physics Institute
X17B3	Insertion Device	XRD, powder XRD, single crystal High pressure research	20-150 keV, 30 and 80 keV monochromatic	FB	BNL-NSLS COMPRES Princeton University Stony Brook University
X17C	Insertion Device	XRD, powder XRD, single crystal High pressure research	5-80 keV	FB	BNL-NSLS COMPRES Princeton University Stony Brook University
X18A	Bend	XRD, powder XRD, single crystal XRD, surface WAXD X-ray reflectivity X-ray scattering, surface WAXS XAS	5-25 keV	FB	BNL-NSLS BNL-Chemistry BNL-Electrochemistry Oak Ridge National Laboratory UOP LLC University of Delaware University of Massachusetts - Department of Chemistry Yeshiva University
X18B	Bend	XAS EXAFS NEXAFS	4.7-40 keV	FB	BNL-NSLS BNL-Chemistry BNL-Electrochemistry Oak Ridge National Laboratory UOP LLC University of Deleware Yeshiva University
X19A	Bend	X-ray scattering, resonant XAS EXAFS NEXAFS	2.1-17 keV	FB	BNL-NSLS BNL-Chemistry BNL-Electrochemistry Oak Ridge National Laboratory UOP LLC University of Deleware Yeshiva University
X19C	Bend	X-ray topography	6-40 keV	PRT	BNL-Instrumentation Fairfield Crystal Technology, LLC Kansas State University SUNY @ Albany Stony Brook University
X20A	Bend	XRD, single crystal WAXD X-ray reflectivity X-ray scattering, surface	4.5-13 keV	PRT	IBM Research Division
X20C	Bend	XRD, time resolved	4-11 keV	PRT	IBM Research Division
X21	Insertion Device	XRD, single crystal XRD, surface WAXD X-ray scattering, magnetic X-ray scattering, resonant X-ray scattering, surface WAXS	6-16 keV	FB	BNL-NSLS Boston University University of Vermont
X22B	Bend	X-ray scattering, liquid	8 keV	PRT	BNL-CMPMSD BNL-CFN

Beamline	Source	Type of Research	Energy Range	Type	Organization
X22C	Bend	XRD, single crystal XRD, surface X-ray reflectivity X-ray scattering, resonant	3-12 keV	PRT	BNL-CMPMSD Massachusetts Institute of Technology Rutgers University
X23A2	Bend	DAFS XAS EXAFS NEXAFS	4.7-30 keV	PRT	National Institute of Standards & Technology
X24A	Bend	XSW Auger spectroscopy EXAFS X-ray fluorescence spectroscopy XPS	1.8-6 keV	PRT	National Institute of Standards & Technology
X24C	Bend	X-ray reflectivity UV absorption spectroscopy XAS	0.006-1.8 keV	PRT	Artep Corporation Naval Research Laboratory (NRL) SFA, Inc.
X25	Insertion Device	MAD Macromolecular crystallography	5-20 keV	FB	BNL-NSLS BNL-Biology
X26A	Bend	InSynC - Education Microdiffraction Imaging X-ray microprobe	3-30 keV	PRT	BNL-Environmental Sciences University of Chicago University of Kentucky
X26C	Bend	MAD Macromolecular crystallography Ultraviolet photo absorption spectroscopy	5-20 keV	PRT	BNL-Biology Cold Spring Harbor Laboratory Stony Brook University
X27A	Bend	X-ray microprobe	4.5-32 keV	FB	BNL-NSLS BNL-Environmental Sciences Stony Brook University - CEMS University of Chicago, Center for Advanced Radiation Sources
X27B	Bend	HARMST	8 - 40 keV	PRT	BNL-Nonproliferation & National Security
X27C	Bend	XRD, time resolved WAXD SAXS WAXS	9 keV	PRT	ExxonMobil Research and Engineering Co. Naval Surface Warfare Center Stony Brook University
X28C	Bend	X-ray Footprinting	Focused White Beam	PRT	Case Western Reserve University
X29A	Insertion Device	MAD Macromolecular crystallography	6-15 keV	PRT	BNL-Biology Case Western Reserve University

SAFETY

"We're proud of the excellent safety record we earned in 2010. It would not have been possible without the hard work, dedication, and experience of the EHS staff and the continuing efforts of our contractors to work more safely."

- Steve Hoey
Manager, Environment, Safety and Health

Photon Sciences EHS Group Expands, Evolves in 2010

Fiscal year 2010 was busy for Environment, Safety, and Health (ESH) staff in the Photon Sciences Directorate, due in no small part to the year-long strategic planning leading up to the reorganization of the directorate at year's end and the continuing rapid growth of NSLS-II.

Photon Sciences ESH already has an excellent safety record under its belt. In 2010, as was the case with the Laboratory as a whole, a strong emphasis was placed on reducing injuries. As a result, there were far fewer accidents among Photon Sciences staff and NSLS-II contractors than in 2009. In fact, in the directorate the only incidents were six first-aid cases, statistics that are well within DOE Office of Science goals. Among the contractors, the injury rates are far better than that of industry in general.

The directorate's exemplary record can be partly attributed to a major "housekeeping" event that took place early in the year, in which staff identified hundreds of safety issues, both large and small. About a third were addressed on the spot, with the remaining items eventually tracked to completion — the most successful housekeeping effort at Brookhaven. Additionally, 18 safety audits conducted throughout the year yielded few findings.

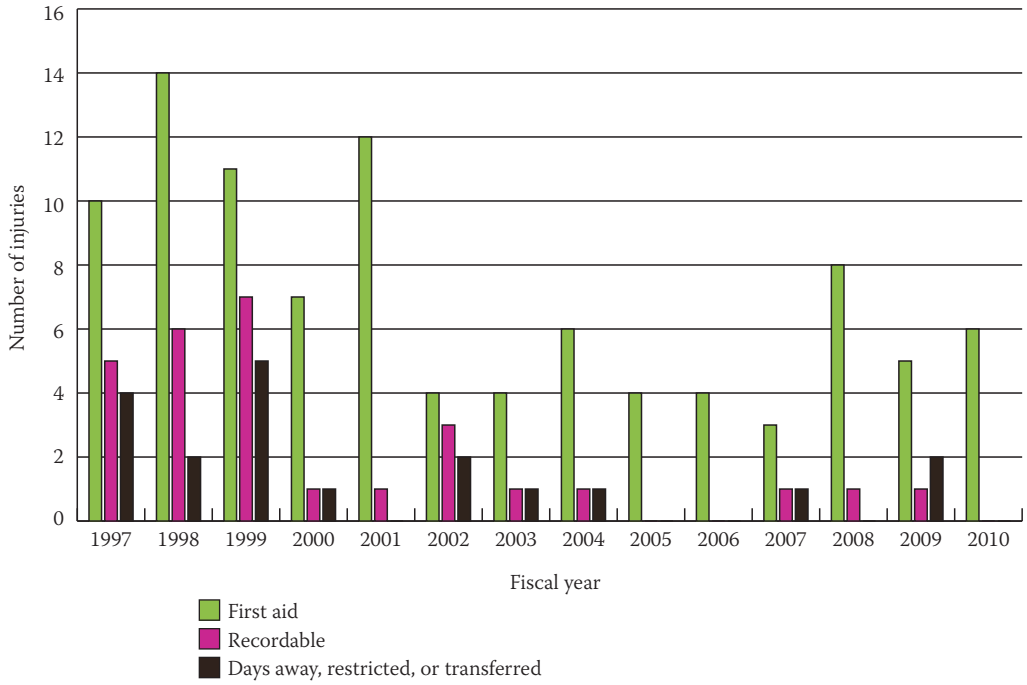
Another notable event was the replacement of a large water-cooling tower on the NSLS roof. The tower needed a new support structure, and staff decided to take the opportunity to swap out the aging tower. This difficult and potentially dangerous task was completed swiftly and without incident.

Radiation safety at NSLS-II was a focus, with a third radiation safety workshop held in June 2010. Experts from Brookhaven and other synchrotrons came together to discuss safety design at the new facility. The design has evolved tremendously since 2008; among its many components will be an advanced system of radiation monitors.

Key steps in the process to ready NSLS-II for operations included completing the Fire Hazards Analysis and the National Emission Standards for Hazardous Air Pollutants assessment, the latter showing that the radiation dose to staff will be well below federal standards. Members of the general public are not expected to be exposed to any radiation when NSLS-II is operating.

Overall, Photon Sciences ESH continues to adapt to the challenges of a new and rapidly growing directorate.

Non-Construction Injury Cases



PEOPLE

We the People

Over 3,000 people carried out the activities of the Photon Sciences Directorate during FY10. This included more than 380 Photon Sciences staff members, 36 employees from other Brookhaven Lab organizations, nearly 340 contractors, and more than 2,200 visiting scientists – or "users" – who came to NSLS during the year to run experiments in fields ranging from biology to materials science.

Among the Photon Sciences staff, 22 percent were scientists, 32 percent were professionals (including engineers), 31 percent were technicians, 11 percent were support staff, and 4 percent were managers.

Staff from other Brookhaven Lab organizations, who typically worked 50 percent or more of their time on Photon Sciences activities, came from groups including the Human Resources Division; the Procurement and Property Management Division; the Community Relations, Education, Government, and Public Affairs Directorate; and the Superconducting Magnet Division.

The largest group among the contractors numbered about 300, who worked on the NSLS-II construction site.

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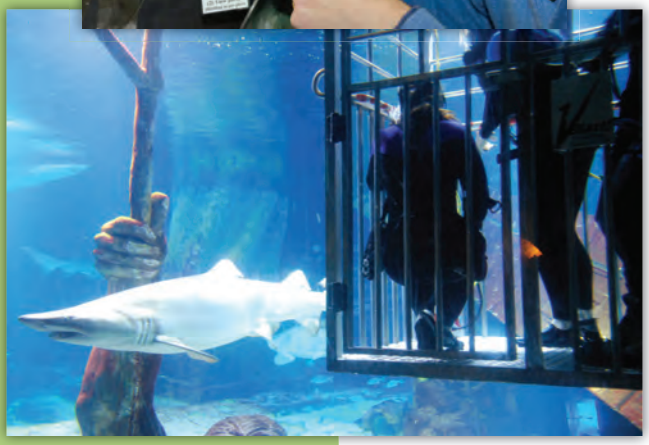


1: Users' Meeting poster session winners with NSLS UEC Chair Bruce Ravel (left): Erik Muller, Louis Piper, Kathryn Dorst, Zhihua Xu, Yimin Mao, and Andrew Ying

2: Photon Sciences employees demonstrate the wow-factor of a Mentos-soda geyser at Take Our Sons and Daughters to Work day

3: University of Chicago geochemist Tony Lanzirotti explains the basics of synchrotrons to local teachers participating in the Introducing Synchrotrons Into the Classroom program.

4: Beamline scientist Allen Orville takes Flat Stanley on a tour of NSLS

5: Physicist Cecilia Sanchez-Hanke and safety engineer Keith Klaus, "winners" of the NSLS-CFN Users' Meeting pledge drive, enjoying their prize: a dip in the shark tank at Atlantis Marine World in Riverhead, NY.

Close-up: NSLS Users

From Alabama to Australia, more than 2,200 visiting scientists from over 400 institutions came to NSLS to conduct their research in FY10. Exactly 700 were new to the facility.

These scientists, known as "users," are awarded beam time by submitting a general user proposal through a peer-reviewed, web-based system. The proposal is rated based on various scientific criteria and can remain active for up to six cycles of operation (about two years).

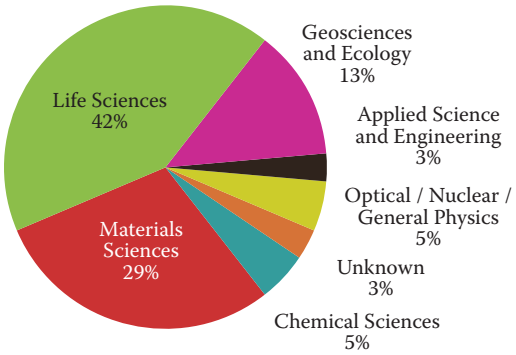
In FY10, about 1,000 requests for beam time were submitted, with about one-third of those requests on new proposals. Beam time is given without charge, as long as the research results are published in open literature. Work that is proprietary in nature is charged on a full-cost recovery basis consistent with U.S. Department of Energy guidelines.

The majority of NSLS users (74 percent) come from academic institutions, and about one third (33 percent) come from New York State. Another third come from locations nearby in the northeastern states. About half of the users are U.S. citizens and almost 27 percent are women.

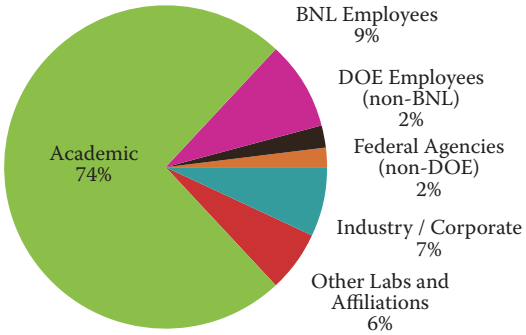
The greatest number of users works in the life sciences field (42 percent), followed by materials science (29 percent). When the number of days spent on experiments is considered, materials science studies make up the largest portion of beam time used (42 percent).

In FY10, almost 40 percent of the researchers working at NSLS were students in undergraduate or graduate programs. About 23 percent of the users were post-doctoral researchers, with faculty members, professional staff, or research scientists making up the balance.

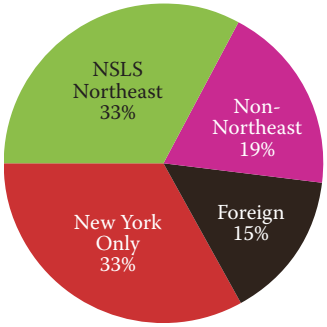
NSLS Users by Field of Research



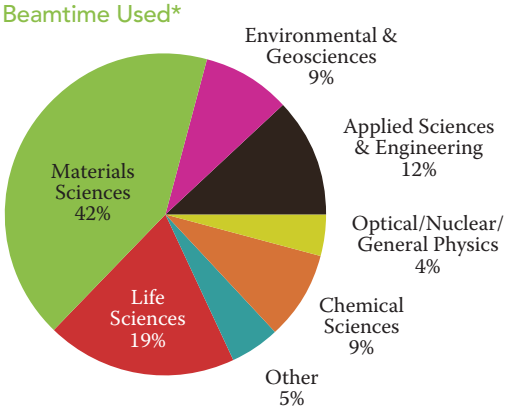
NSLS Users by Affiliation



Geographical User Distribution



Beamtime Used*



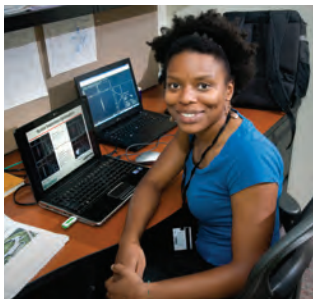
* Based on running times from Safety Approval Forms

Aspiring Scientists and Engineers Spend Summer at NSLS, NSLS-II

More than 40 college students and professors spent their summer at Brookhaven Lab to work on a wide variety of science and engineering projects at NSLS and NSLS-II. The visitors — 26 students and two Faculty and Student Teams (FaST) program professors at NSLS and 14 students at NSLS-II — worked alongside Photon Sciences employees in areas ranging from the study of Alzheimer's disease to the development of new software and instrumentation. Students also had the opportunity to attend scientific lectures, tour Brookhaven's research facilities, and participate in numerous social activities.

The Laboratory was especially delighted to host 13 students from the GEM program, which is by far the largest number of GEM students ever at BNL. Of these, 11 worked at NSLS-II, one at the Center for Functional Nanomaterials, and one in the Collider-Accelerator Department. GEM stands for National Consortium for Graduate Degrees for Minorities in Engineering and Science, Inc.

In the GEM Fellow Technical Presentation Competition in Virginia at the end of the summer, two NSLS-II GEM students took top honors: Rafael Lozano, a first-year graduate student in aerospace engineering at the Georgia Institute of Technology, came in first overall, and Niaja Farve, who started graduate school at the Massachusetts Institute of Technology in the fall, came in third. Under the supervision of Evgueni Nazaretski, Lozano worked on nanopositioning R&D for the hard x-ray nanoprobe beamline at NSLS-II, designing the new end station microscope. Farve worked with scientists Juergen Thieme and Vincent DeAndrade to perform ray tracing for the future submicron-resolution x-ray spectroscopy beamline at NSLS-II.



Left: 2010 Photon Sciences Directorate summer students

Right, top: Rafael Lozano, first-place winner in the GEM Fellow Technical Presentation Competition

Right, bottom: Niaja Farve, third-place winner in the GEM competition

A Little Help from our Friends

The Photon Sciences (PS) directorate frequently seeks advice from a number of external committees made up of users, reviewers, and experts in a wide range of scientific fields.

The Users' Executive Committee provides a forum for ongoing, organized discussions between representatives of the NSLS user community and the management and administration of PS, Brookhaven National Laboratory, funding agencies, Congress, and other synchrotron user groups. Its goal is to communicate current and future needs, concerns, and trends, and to disseminate information about plans for NSLS, NSLS-II, and Brookhaven Lab. In addition to regular members, the UEC appoints Special Interest Group (SpIG) representatives, who are divided into areas of common concern.

In March, two of the directorate's committees, the NSLS Science Advisory Committee and the NSLS-II Experimental Facilities Advisory Committee, were replaced with the Photon Sciences Science Advisory Committee (SAC). The SAC advises the Associate Laboratory Director for Photon Sciences on all scientific and policy issues related to the full and effective use of NSLS and NSLS-II and on future developments required to achieve the highest possible scientific productivity of both facilities.

As part of the peer-review process of general user proposals, the Proposal Review Panels (PRPs) review and rate the proposals within their scientific area. Members are drawn from the scientific community and usually serve a two-year term. Each PRP has an appointed chair, who is part of the Proposal Oversight Panel, or POP, with a few other select members. The POP reviews proposals that might need special attention due to use of multiple techniques or conflicts in scores.

In addition to the SAC, staff members working on the NSLS-II Project consult with three groups: the NSLS-II Project Advisory Committee (PAC), the Accelerator Systems Advisory Committee (ASAC), and the Conventional Facilities Advisory Committee (CFAC).

The PAC reviews the progress of the NSLS-II Project on matters related to project planning, execution, management, and safety. It identifies issues whose resolution is critical to the success of the project in meeting project performance, cost, and schedule goals, and provides continuity of oversight until the completion of the project.

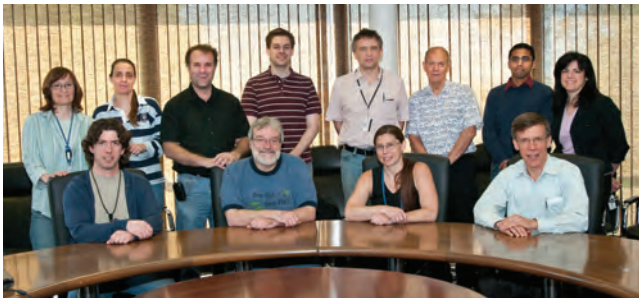
The ASAC is composed of external experts trained in accelerator physics and engineering who are familiar with the design, construction, and operations of major accelerator systems. This group provides guidance on technical choices, trade-offs, and decisions; value engineering; measures to improve availability and reliability of operations; diagnostics and controls; and other related issues.

The CFAC is comprised of external experts trained in conventional construction, most of whom have had extensive experience in designing and constructing conventional facilities and the supporting infrastructure associated with major scientific user facilities. This group provides advice on the development of the improvements to land, conventional construction, and utilities systems required to deliver the maximum benefit to users.

The members of these valuable groups are listed in the following pages.

Top: Science Advisory Committee

Bottom: Users' Executive Committee



Users' Executive Committee

Chair Tony Lanzirotti, *University of Chicago*
Vice Chair Simon Billinge, *Columbia University*
Past Chair Bruce Ravel, *National Institute of Standards and Technology (NIST)*
General Member Jay Bass, *University of Illinois*
General Member Jen Bohon, *Case Western Reserve University*
General Member Dan Fischer, *NIST*
General Member David Mullins, *Oak Ridge National Laboratory*
Ex-Officio Lisa Miller, *BNL*
Ex-Officio Kathy Nasta, *BNL*
Ex-Officio Qun Shen, *BNL*

UEC Special Interest Group Representatives

Bio. Crystallography & Diffraction Annie Heroux, *BNL*
High Pressure Michael Vaughan, *Stony Brook University (SBU)*
Imaging Paul Northrup
Industrial Users Jean Jordan-Sweet, *IBM Research Division*
Infrared Users Randy Smith, *BNL*
Magnetism Cecilia Sanchez Hanke, *BNL*
Students & Post Docs Alvin Acerbo, *SBU*
Topography Michael Dudley, *SBU*
UV Photoemission & Surface Science Sanjaya Senanayake, *BNL*
EXAFS Anatoly Frenkel, *Yeshiva University*

Science Advisory Committee

Simon Bare, *UOP, LLC*
Murray Gibson, *Northeastern University*
Ernie Hall, *General Electric Global Research*
Jerry Hastings, *SLAC National Accelerator Laboratory*
Russell Hemley, *Carnegie Institution of Washington*
John Hemminger, *University of California, Irvine*
Keith Hodgson (Chair), *SLAC National Accelerator Laboratory*
Leemor Joshua-Tor, *Cold Spring Harbor Laboratory*
Steve Kevan, *University of Oregon*
Sine Larsen, *University of Copenhagen*
Gerd Materlik, *Diamond Light Source*
Simon Mochrie, *Yale University*
Harald Reichert, *European Synchrotron Radiation Facility*
Janet Smith, *University of Michigan*
Friso van der Veen, *Swiss Light Source*
Pierre Wiltzius, *University of California, Santa Barbara*

Proposal Review Panels

IR/UV/Soft X-ray Spectroscopy: Chemical Sciences/Soft Matter/Biophysics
Benjamin DeKoven, *X-Lubes, Inc.*
Daniel Fischer (Chair), *NIST*
Mary Gilles, *Lawrence Berkeley National Laboratory*
Joseph Lenhart, *Army Research Laboratory*
Robert Lodder, *University of Kentucky*
Gary Mitchell, *Dow Chemical Company*

IR/UV/Soft X-ray Spectroscopy: Magnetism/ Strongly Correlated Electrons/Surface
Robert Bartynski (Chair), *Rutgers University*
Alexander Moewes, *University of Saskatchewan*
David Mullins, *Oak Ridge National Laboratory*
Robert Opila Jr, *University of Delaware*
Boris Sinkovic, *University of Connecticut*
Jiufeng Tu, *City University of New York*
Tonica Valla, *BNL*

Imaging & Microprobes: Biological & Medical
Fulvia Arfelli, *University of Trieste/INFN*
Leroy Chapman, *University of Saskatchewan*
Paul Dumas, *Soleil Synchrotron*
Meghan Faillace, *Mount Sinai School of Medicine*
Barry Lai (Chair), *Argonne National Laboratory*
Andreana Leskovjan, *SBU*
Irit Sagi, *Weizmann Institute of Science*
Franz Stefan Vogt, *Argonne National Laboratory*
Samuel Webb, *SLAC National Accelerator Laboratory*
Gayle Woloschak, *Northwestern University*

Imaging and Microprobes: Chemical and Material Sciences
Harald Ade (Chair), *North Carolina State University*
David Black, *Topographix*
Darren Dale, *Cornell University*
Paul Evans, *University of Wisconsin*
Mark Rivers, *University of Chicago*
Paul Zschack, *Argonne National Laboratory*

Imaging and Microprobes: Environmental and Geosciences
Don Baker, *McGill University*
David Black, *Topographix*
Darren Dale, *Cornell University*
George Flynn, *State University of New York at Plattsburgh*
Matthew Ginder-Vogel, *Calera*
Keith Jones (Chair), *BNL*
Mark Rivers, *University of Chicago*
Donald Ross, *University of Vermont*

InSynC – Education
Scott Calvin, *Sarah Lawrence College*
Jonathan De Booy, *Australian Synchrotron*
Tracy Walker, *Canadian Light Source*

Industrial IR/UV/Soft X-ray Spectroscopy
Benjamin DeKoven, *X-Lubes, Inc.*
Daniel Fischer, *NIST*
Gary Mitchell, *Dow Chemical Company*

Industrial Imaging & Microprobes
Michael Feser, *Xradia Inc.*
Jeffrey Gillow, *Arcadis G&M Inc.*
Matthew Ginder-Vogel, *Calera*
Karina Lange, *Canadian Nuclear Safety Commission*
Christopher Ryan, *Commonwealth Sci.& Indust. Research Org.*

Industrial Powder/Single Crystal Crystallography
Thomas Blanton, *Eastman Kodak Company*
James Kaduk, *Poly Crystallography Inc.*
Peter Stephens, *SBU*

Industrial X-ray Scattering
Benjamin Hsiao, *SBU*
Christian Lavoie, *IBM Research Division*
Paul Stevens, *ExxonMobil Research and Engineering Co.*

Industrial X-ray Spectroscopy
In Tae Bae, *Dura Cell Technical Center*
Simon Bare, *UOP, LLC*
Douglas Hunter, *Westinghouse Savannah River Co.*
Bruce Ravel, *NIST*

Macromolecular Crystallography
Steven Almo, *Albert Einstein College of Medicine*
Alex Bohm (Chair), *Tufts University*
Olga Boudker, *Cornell University*
Barnali Chaudhuri, *Hauptman-Woodward Medical Research Inst.*
Ashley Deacon, *SLAC National Accelerator Laboratory*
Annie Heroux, *BNL*
Xiangpeng Kong, *New York University*
Steven Roderick, *Albert Einstein College of Medicine*
Brenda Schulman, *St. Jude Children's Research Hospital*

Methods and Instrumentation
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Ali Khounsary, *Argonne National Laboratory*
Ralf Hendrik Menk, *Sincrotrone Trieste*
Thomas Rabedeau, *SLAC National Accelerator Laboratory*
Ruben Reininger, *BNL*
Anthony Warwick, *Lawrence Berkeley National Laboratory*

Powder / Single Crystal Crystallography
Emil Bozin, *Columbia University*
Andrew Campbell, *University of Chicago*
Karena Chapman, *Argonne National Laboratory*
Yu-Sheng Chen, *University of Chicago*
Przemyslaw Dera, *University of Chicago*
James Kaduk (Chair), *Poly Crystallography Inc.*
Volker Kahlenberg, *University of Innsbruck*
Peter Khalifah, *BNL*
Stefan Kycia, *University of Guelph*
Peter Lee, *Argonne National Laboratory*
Wendy Panero, *Ohio State University*
Peter Stephens, SBU

Structural Biology in Solution
Joanna Krueger (Chair), *University of North Carolina*
Bryan Nixon, *Pennsylvania State University*
Peter Prevelige, *University of Alabama*
Steven Roderick, *Albert Einstein College of Medicine*
Bianca Sclavi, *Centre National de La Recherche Scientifique*
Brian Shilton, *University of Western Ontario*
Hirotsugu Tsuruta, *Stanford University*

X-ray Scattering: Magnetism / Strongly Correlated Electrons / Surface
Peter Abbamonte, *University of Illinois at Urbana-Champaign*
Kenneth Finkelstein, *Cornell University*
Karl Ludwig (Chair), *Boston University*
Peter Hatton, *University of Durham*
Christopher Marrows, *University of Leeds*
George Srajer, *Argonne National Laboratory*
Trevor Tyson, *New Jersey Institute of Technology*
Gerrit Van Der Laan, *Diamond Light Source*

X-ray Scattering: Soft Matter and Biophysics
Masafumi Fukuto, *BNL*
Randall Headrick, *University of Vermont*
Benjamin Hsiao (Chair), *SBU*
Huey Huang, *Rice University*
Detleff-Matthias Smilgies, *Cornell University*

X-ray Spectroscopy: Biological, Environmental and Geosciences
Martine Duff, *Westinghouse Savannah River Co.*
Graham George, *University of Saskatchewan*
Douglas Hunter, *Westinghouse Savannah River Co.*
Keith Jones, *BNL*
Satish Myneni (Chair), *Princeton University*
Bruce Ravel, *NIST*

X-ray Spectroscopy: Chemical and Material Sciences
Simon Bare, *UOP, LLC*
Scott Calvin, *Sarah Lawrence College*
Anatoly Frenkel, *Yeshiva University*
Steve Heald, *Argonne National Laboratory*
Jean-Pascal Rueff, *Synchrotron SOLEIL*
Tsun-Kong Sham, *University of Western Ontario*
Trevor Tyson (Chair), *New Jersey Institute of Technology*
Stephen Wasserman, *Eli Lilly and Company*

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Jonathan Hanson, *BNL*
Subramanyam Swaminathan, *BNL*
Harald Ade, *North Carolina State University*
Robert Bartynski, *Rutgers University*
Alex Bohm, *Tufts University*
Daniel Fischer, *NIST*
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James Kaduk, *Poly Crystallography Inc.*
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Antonio Lanzirotti, *University of Chicago*
Joanna Krueger, *University of North Carolina*
Peter Stephens, *SBU*
Trevor Tyson, *New Jersey Institute of Technology*
Satish Myneni, *Princeton University*

NSLS-II Project Advisory Committee
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Gene Desaulniers *(retired)*
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Suzanne Herron, *Oak Ridge National Laboratory*
Michael Rowe, *NIST (retired)*
Les Price, *Oak Ridge National Laboratory (retired)*
Albin Wrulich, *Paul Scherrer Institute*

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Douglass Rowland, *Oak Ridge National Laboratory*
Elaine McCluskey, *Fermi National Accelerator Laboratory*
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