BROOKHAVEN NATIONAL LABORATORY

NEWSLETTER

national synchrotron light source

Spring 2005

Hunting the RNA "Slicer"

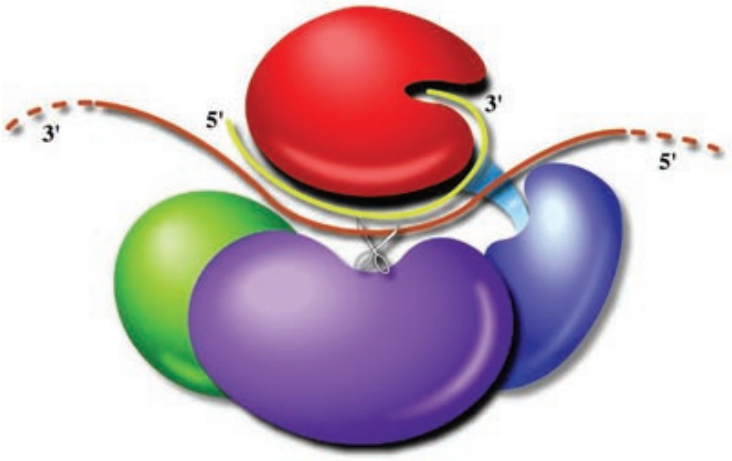
NSLS Users May Have Found a Key Player in RNA Interference

Laura Mgrdichian, NSLS Science Writer

As the result of work done at the NSLS, scientists from Cold Spring Harbor Laboratory have very likely determined the identity of a sought-after protein that is vital to RNA interference (RNAi). The results appeared in the September 3, 2004, issue of *Science*.

RNAi is fundamental cellular process intimately involved in the development and virus-fighting ability of all organisms, as well as gene expression – how genes produce certain cell features. The researchers' result, the crystal structure of the protein, will significantly impact the field of biology by helping to illuminate the details of these mechanisms.

Before the protein was identified, biologists only knew that there should be a protein, dubbed the "Slicer," that performed a critical role in RNAi. It received this nickname for the function the scientists suspected it carried out: slicing, or cleaving, strands of messenger RNA into pieces, much like a pair of molecular "scissors." Messenger RNA is the type of RNA that decodes the information contained in DNA (i.e. genes) and carries it out of the cell nucleus, where it is used to synthesize proteins. The Slicer is one component of a large multi-protein structure, called the RNA-induced silencing complex (RISC), that "interferes" with messenger RNA's mission.



A schematic depiction of the model for siRNA-guided messenger RNA cleavage. The siRNA binds with its 3' end in the cleft in the globular domain. The 5' end is predicted to bind near the other end of the cleft. The messenger RNA strand comes in between the crescent's N-terminal and globular domains and out between the globular domain and the crescent's middle domain.

This research team is the first to discover very convincing evidence that a certain protein is, in fact, the Slicer. The protein is known as Argonaute.

"The crystal structure of Argonaute contained a clue that led us to identify it as the Slicer," said Leemor Joshua-Tor, a structural biologist and the study's lead researcher. "We observed that an important structural feature on Argonaute was very similar to that of another enzyme already known to cleave RNA."

The group found that Argonaute is composed of a large crescent-shaped base and a smaller globular region that sits over it, tethered by

INSIDE THIS EDITION

Leemor Joshua-Tor (left) and Greg Hannon (© Miriam Chua, 2004).

a thin stalk-like region. The crescent has own sub-structure, made up of three distinct parts, or "domains" – a center domain and two outer ones.

Based on these features, Joshua-Tor and her colleagues postulated how Argonaute might act as the Slicer. In their scenario, a strand of "small interfering" RNA (siRNA), which is a short type of RNA created earlier in the interference process, binds to Argonaute and guides it to a complementary strand of messenger RNA. The siRNA positions the messenger RNA in the groove created by Argonaute's crescent and globular segments. Once in place, the crescent's "PIWI" domain cleaves the messenger RNA, leaving the siRNA intact.

"This is an important result, but many questions still remain," said Joshua-Tor. "For example, we still do not know how Argonaute proteins participate in developmental processes."

Gene silencing during RNAi (the act of blocking gene expression) may sound destructive, but the process can prevent messenger RNA from carrying out the orders of potentially malicious genes – genes for defects, for example. RNAi also appears to play an important role in normal organ function. Currently, biologists are experimenting with ways to silence specific genes for medical purposes.

Joshua-Tor and her colleagues, including student researcher Ji-Joon Song, collected data at NSLS beamline X25 and later used the data to determine Argonaute's structure.

Using a technique called protein crystallography, they directed a beam of x-rays at a crystal of Argonaute protein and used a detector to collect the x-rays as they scattered away from the atoms in the crystal. The researchers then analyzed this pattern, which is unique to Argonaute, to create a three-dimensional model of the protein.

Ji-Joon Song (left) and Stephanie K. Smith

This research was funded by Cold Spring Harbor Laboratory. Ji-Joon Song is a Bristol-Myers Squibb fellow.

Cold Spring Harbor Laboratory researchers Gregory J. Hannon and Stephanie K. Smith also participated in this research.

EVENTS

X6A Workbench Provides Hands-On Training in Synchrotron Crystallography

Vivan Stojanoff, BNL-NSLS

Beamline X6A, the NIGMS facility at the National Synchrotron Light Source, is offering comprehensive hands-on training in synchrotron data collection and analysis for biophysicists, biochemists and molecular biologists.

The first "X6A Workbench: Advanced Structural Biology Tools" workshop took place this year from March 1-4, 2005. Participants practiced cryogenic protection of their samples and learned how to load sample cassettes for the X6A automounter. The program followed with hands-on crystallography data collection and analysis. Molecular replacement and Multiwavelength Anomalous Diffraction (MAD) software suites were discussed.

Participants screened their own samples and applied the new data analysis concepts introduced during the workshop.

The X6A workbench is regularly offered throughout the year. The next two workshops are scheduled for April 26-29 and July 12-15, 2005. For more details and registration information, go to: http://protein.nsls.bnl.gov/news/workbench.php.

Participants in the first "X6A Workbench: Advanced Structural Biology Tools" workshop: (sitting, from left) Caroline LaFleur and Michael Hickey; (standing, from left) Renae Ryan, Marc Allaire, Vivian Stojanoff, Raimund Fromme, Ingo Grotjohann, Chuanyong Jing, and Jean Jakoncic.

Notes from the UEC

Larry Shapiro, Users' Executive Committee Chair
Columbia University

This will be my last newsletter as UEC chair, as I pass this role on to Peter Stephens (Stony Brook University) in May. I have really enjoyed representing the NSLS user community during a very exciting time, and look forward to an exciting future for the NSLS.

The UEC continues to take steps to help our political representatives understand the importance of the NSLS to science in the Northeast, and NSLS-II to the continuation of great science here in the future. Recently, I met with Long Island Congressman Timothy Bishop to stress the importance of NSLS and ask for his active support. Congressman Bishop understands the importance of BNL to Long Island and New York, and understands that the NSLS is extremely important to the Lab.

The UEC has also started to arrange a trip to Washington, scheduled for April, in order to meet with legislators and legislative staff. This trip, as is the custom, will be made jointly with user representatives from the other DOE synchrotron facilities, and will underscore the national importance of synchrotron research.

The 2005 NSLS Users' Meeting will be held this year from May 23-25, which is rapidly approaching. In the last few years, we've had record attendances for this meeting, and we have lots of excitement planned for this year too, including keynote speaker, Henk Schenk from the University of Amsterdam, who will speak on the science of chocolate. Workshops this year will include: "Nanomagnetism: Materials and Probes," " Imaging Nanoscale Structure in Biominerals," "The Impact of Cryogenic Specimen Automounters on the Future of Macromolecular Crystallography," "Spectroscopic Studies of Nanoscaled Systems," "Application of Small Angle X-Ray Scattering to Biological Structures," "In-situ Kinetic Analyses in Environmental Systems, " and "Electrical Safety in the Research Community." A poster detailing this year's meeting is in the center of this Newsletter and complete information can be found on the NSLS homepage.

It is also the time of year to vote for a new set of Users' Executive Committee (UEC) members and Special Interest Group (SpIG) representatives. In addition, we are now collecting nominations for this year's UEC Community Service Award. Nominations and voting are online and can be found on the UEC website at http://www.nslsuec.org. Please make your vote count!

Being UEC chair this year has been an amazing learning experience for me. Immersion in NSLS science gave me new and enormous respect for the quality of science and the scientists who use the NSLS. No group of scientists could have proved their worth better than ours, and we can realistically hope that past successes and a great future vision will lead to a favorable decision to go forward with NSLS-II.

UEC Nominees

Steve Almo
Professor
Depts. of Biochemistry and Physiology & Biophysics
Albert Einstein College of Medicine

Chris Jacobsen
Professor
Dept. of Physics & Astronomy
Stony Brook University

Liang Tong
Professor
Dept. of Biological Sciences
Columbia University

Chris Cahill
Assistant Professor
Dept. of Chemistry
George Washington University

Troy Rasbury
Assistant Professor
Dept. of Geosciences
Stony Brook University

Hanno zur Loye
Professor
Dept. of Chemistry and Biochemistry
University of South Carolina

Please vote online at: http://www.nslsuec.org/elections/uec-vote.asp

Short Course Participants Learn the Value of Synchrotron Light for Powder Diffraction

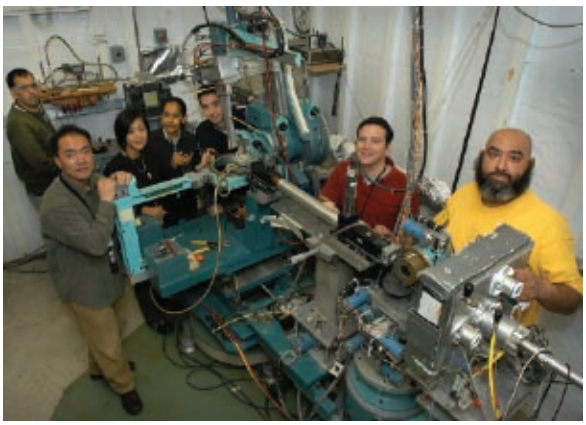
Christie Nelson, BNL-NSLS

Participants in the High Resolution Powder Diffraction Data Collection and Analysis Course

Fifteen participants recently attended the High Resolution Powder Diffraction Data Collection and Analysis Short Course, which was held at the NSLS from January 25-27, 2005. The three-day course consisted of lectures, guest talks, hands-on data collection, and data analysis, and was co-organized by Peter Stephens (Stony Brook Univ.), Christie Nelson (NSLS), and Chi-Chang Kao (NSLS), with administrative support provided by Corinne Messana (NSLS).

The 15 participants included graduate students, post-docs, and scientists from national labs and universities. While most of the students were familiar with lab-based powder diffraction techniques, very few had synchrotron experience. The participants were all quite eager to learn about the impact that synchrotron-based powder diffraction could have on their own research.

The lectures were presented by Peter Stephens, Pat Woodward (Ohio State Univ.), and John Parise (Stony Brook Univ.), and covered the basic physics of powder diffraction, experimental aspects of data collection, Rietveld refinement, and indexing. In addition, specialized talks on cutting edge research on high-pressure, high-temperature, and time-resolved powder diffraction were given by guest speakers Yongjae Lee (BNL-CMP), Cam Hubbard (ORNL), and Jonathon Hanson (BNL-Chemistry), respectively.



Setting up at beamline X7A

The hands-on data collection component of the course was carried out on NSLS beamlines X3B1, X7A, and X14A, with beamline instructors Peter Stephens, Yongjae Lee, and Jianming Bai (ORNL), respectively. The participants first learned about beamline operation and sample preparation, and then collected data from a corundum standard. Next, the participants collected high-resolution data from samples of interest in their own research projects.

In addition to the lectures and data collection, the participants also spent time learning about data analysis techniques. "Homework" assignments included refining the corundum standard data as well as additional data sets, and then students tackled the data obtained from their own samples. The participants were greatly aided in the completion of these tasks by their three lecturers.

At the end of the intensive three-day course, the participants left with a foundation of knowledge about applying high resolution powder diffraction to their own research projects. Many expressed interest in becoming NSLS users, and we look forward to seeing them back here soon.

Data collection at beamline X3B1

The organizers would like to thank the lecturers, guest speakers, beamline instructors, Elaine Dimasi (NSLS), Jae-Hyuk Her (Stony Brook Univ.), Corinne Messana, and the NSLS User Administration Office and safety staff for all of their help in making the short course such a success.

Unique Global Light Source Website Launched

On February 17th, the international light source community launched the first website dedicated to providing the media, general public, and scientific community with the latest news and information on the world's accelerator-driven light sources (synchrotrons and free-electron lasers) and the science they produce.

The web site – *www.lightsources.org* – was developed and is jointly maintained by the Light Source Communicators Group, whose members represent the world's light source facilities in Europe, North America, and Asia. Funding for the project is provided by science funding agencies of many nations.

Visit www.lightsources.org for the latest news releases on cutting-edge areas of advanced light source applications for science and technology from facilities around the world.

Anyone can subscribe free of charge to "News Flash," which will email subscribers when news releases and other light source information is posted to the website. Also available on the website are an image bank of light source-related photos and graphics, clippings of news stories, links to light source facility websites, and relevant articles and presentations.

Educators will find links to websites relating to light sources and the science conducted at these facilities. Researchers can find specific information regarding each light source facility, including job opportunities and events related to science outreach activities.

Sponsors of lightsources.org:

- Advanced Light Source (ALS)
- Advanced Photon Source (APS)
- Canadian Light Source (CLS)
- ELETTRA (Sincrotrone Trieste)
- European Synchrotron Radiation Facility (ESRF)
- Hamburger Synchrotronstrahlungs Labor (HASYLAB)
- National Synchrotron Radiation Research Center (NSRRC)
- National Synchrotron Light Source (NSLS)
- Photon Factory
- Pohang Light Source (PLS)
- Stanford Synchrotron Radiation Laboratory (SSRL)
- SPring-8
- Synchrotron Radiation Center (SRC)
- Synchrotron Ultraviolet Radiation Facility (SURF III)
- Swiss Light Source (SLS)
- The Free-Electron Laser at the Thomas Jefferson National Accelerator Facility (JLab)

Groundbreaking for Research Support Building at Brookhaven Lab

Diane Greenberg, BNL Media & Communications Office

On March 10th, Brookhaven National Laboratory held a groundbreaking ceremony for the construction of the new 65,000-square-foot Research Support Building.

The new Research Support Building will consolidate frequently visited administrative and support functions in a single location to provide more efficient administrative services to Brookhaven employees and visiting scientists.

An artist's rendering of the new Research Support Building, which is set to be completed in the fall of 2006.

"The Research Support Building is the first to be constructed under Brookhaven Lab's master plan for its 5,300-acre site, in which we envision Brookhaven Avenue – where the new building will be centrally located – as the 'Main Street' of the Laboratory," said Project Manager Gregory Flett. "We expect the building to be completed in the fall of 2006."

The Research Support Building tops New York State requirements for energy efficiency by 15 percent, and the structure will be considered "green," or environmentally friendly, based on the U.S. Green Building Council's Leadership in Energy & Environmental Design, also known as LEED, rating system. Also, the building complies with National Environmental Policy Act requirements.

The Research Support Building will house a number of staff and user services, including the Housing, Transportation & Travel Office, the Identification Badging Office, the Community, Education, Government & Public Affairs Office, and a branch of the Teachers Federal Credit Union.

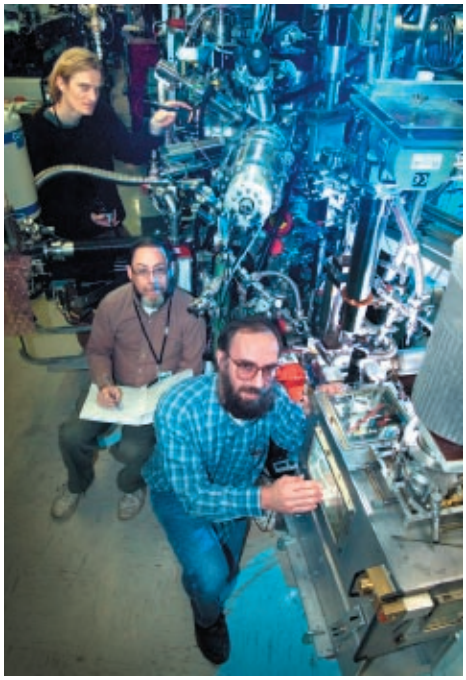
EnviroSuite: Environmental Science at the NSLS

Paul Northrup, BNL-Environmental Sciences

Created in response to rapidly growing interest in environmental synchrotron science, the EnviroSuite Strategic Initiative is designed to support and develop a suite of state-of-the-art resources at the NSLS for molecular environmental science research. Its mission is to optimize and expand synchrotron-based techniques for exploring environmental questions, to establish substantial involvement in several beamlines to bring a multifaceted approach to complex environmental processes, and to introduce new users to these capabilities at the NSLS. EnviroSuite now provides a unified voice for the diverse community of environmental science users.

EnviroSuite is coordinated by the Environmental Research and Technology Division of BNL's Environmental Sciences Department, and is funded by the Office of Biological & Environmental Research, Environmental Remediation Sciences Division (BER:ERSD), in DOE's Office of Science. Similar programs have been initiated at all four DOE synchrotron facilities. Its BNL core consists of a number of environmental scientists, who work closely with the NSLS and with CEMS, the NSF/DOE-funded Center for Environmental Molecular Science based at Stony Brook *(www.cems.stonybrook.edu)*.

EnviroSuite is taking an active role in both PRT and NSLS facility beamlines, in order to direct the course of beamline development and harness the resources to conduct leading research. As a result, both capital funding and scientific staff have been brought to the NSLS. Some of these are described in more detail below. In addition, a key goal of the EnviroSuite program is to establish the framework for multi-beamline studies, such as combining bulk EXAFS with microspectroscopy and imaging of elemental and species distributions.



Environmental scientists (from left) Jeff Fitts (EnviroSuite Coordinator), Mark Fuhrmann (X11 Spokesperson), and Paul Northrup (X15B Spokesperson) at the X15B end station.

NSLS facility beamline X27A, a new hard x-ray microprobe beamline, was highlighted in the December 2004 Newsletter. It will have a 5x15 μm spot size at 3.5 - 32 keV, a 13-element solid state detector, and control software modeled after the beamline X26A system. EnviroSuite collaborated with the NSLS, X26A, and CEMS for the design and commissioning of X27A, and provided the detector. This beamline will greatly increase available microbeam resources at the NSLS. Environmental applications include x-ray fluorescence microanalysis of trace elements, mapping of their distribution, and microspectroscopy.

Beamline X11 is one of the most scientifically productive and historically important beamlines at the NSLS, being used primarily for bulk EXAFS experiments. It has an unfocused beam (0.5x10 mm), and operates in the energy range from 4.5 - 35 keV. It is versatile, and can accommodate a variety of sample types as well as in-situ studies. EnviroSuite will be adding a new 13-element Ge detector to X11A, to enhance its capabilities for low-concentration and otherwise challenging environmental samples. Detector capability at beamline X11B will also be upgraded.

Beamline X15B is designed for low- to medium-energy bulk and surface x-ray absorption spectroscopy (optimized for 1.7 - 5 keV). It has a 1 mm focused spot size, and can address samples in ultra-high vacuum or air/He atmosphere. Current research includes phosphorus, sulfur, and silicon K-edge, cadmium L-edge, and uranium and lead M-edge spectroscopy.

Beamline X1A is a soft X-ray beamline used for scanning transmission x-ray spectromicroscopy. Its primary emphasis is on organic materials at the carbon and oxygen absorption edges. With a resolution of ~30 nm, X1A is well suited for imaging molecular chemical features on a sub-cellular scale, such as for research exploring mechanisms of biotransformation of radioactive and toxic species. Recent upgrades include a BER:ERSD-funded laser interferometer.

EnviroSuite can provide guidance for new and experienced General Users with environmental science research at these and other beamlines. BNL Environmental Science Department resources include laboratory facilities for handling radioactive and hazardous materials and wastes, and for sample preparation. Experimental protocols are being developed to facilitate safe handling and analysis of samples containing radionuclides. For further information, see the EnviroSuite and NSLS web pages (*www.bnl.gov/envirosuite, www.nsls.bnl.gov*) or contact Jeff Fitts (fitts@bnl.gov).

High-Resolution Terahertz Spectroscopy in a Magnetic Field

Laszlo Mihaly[1] and G. Lawrence Carr[2]
[1]Stony Brook University; [2]BNL-NSLS

Over the past few years a new magneto-optical facility has been developed at NSLS beamline U12IR. The main components are an Oxford Instrument superconducting magnet and a Bruker IFS 125HR high-resolution spectrometer. The principal reason for using the synchrotron source in far IR spectroscopy is the brightness advantage over a conventional light source -- depending on the frequency range and on the sample geometry, the synchrotron results in a factor of 50 - 200 gain in the intensity, making a vast array of new measurements possible.

The Oxford Instruments magnet, installed next to the Bruker IFS 125HR spectrometer. The stainless steel tubes contain the optical coupling to the VUV-IR ring and between the spectrometer and the magnet.

The Bruker spectrometer is essentially an interferometer where spectral resolution is proportional to the available path difference (between the two interferometer "arms"). This particular spectrometer has an extremely long path difference, yielding a 0.001 cm^{-1} (0.125 μeV) resolution. The available spectral range is from 5 cm^{-1} (0.63 meV) to over 7000 cm^{-1}. The magnet can produce fields up to 16 Tesla and its 20-liter He reservoir has a hold time of nearly one week. A set of three wedged single-crystal quartz windows at the bottom provide optical access to the sample from below, along the vertical axis of the magnet. The sample temperature can be varied between 1.8 K and room temperature.

The facility's first results were published on $LaMnO_3$, a well-known antiferromagnet. Other projects in progress include: the study of the single molecular magnet Mn_{12}-acetate (in collaboration with Myriam Sarachik, City College of New York), spin resonance on $NaNiO_2$ (with Sophie De Brion, Grenoble HMFL), the investigation of correlated magnetic systems, including $LiCu_2O_2$ (with Laszlo Forro, EPFL, Lausanne), and magneto-optical studies on superconductors, including carbon-doped MgB_2.

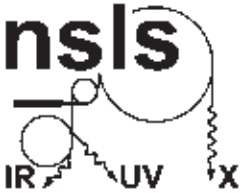
A 10T Superconducting Magnet for Magneto-Structural and Magneto-Electronic Research and Education

T.A. Tyson[1], J. Budnick[2], M.C. Croft[3], V.G. Harris[4], and C.-C. Kao[5]
[1]NJIT; [2]University of Connecticut; [3]Rutgers University; [4]formerly NRL; [5]BNL-NSLS

A horizontal-field, split-coil superconducting magnet has become available for magneto-structural and magneto-electronic research at the NSLS. The magnet can operate from 1.6 to 300 K and over the field range 0 to 10 T. The horizontal field enables x-ray absorption measurements with linearly polarized x-rays with the electric field of the beam parallel to or normal to the magnetic field. Care was taken in the design to ensure that the samples can be measured in transmission mode for energies down to 5 keV (and in small steel hutches).

In general, this magnet is being used to study the lattice-spin coupling in complex materials. It was designed to be used on beamlines X11A, X19A, X21A, and X23B for structural measurements (x-ray absorption fine structure and powder x-ray diffraction) in magnetic fields. With the use of a quarter-wave plate, hard x-ray circular dichroism measurements on these beamlines will be feasible. With a differential pumping configuration, a future upgrade will make possible x-ray magnetic circular dichroism (XMCD) measurements on beamlines X13A and U4B. This will enable the study of magnetism in hard magnets as well as the induced moments on oxygen sites in metal oxide systems. Optical access is possible by replacing the kapton windows with quartz windows and/or replacing the variable temperature insert windows and external windows with all-quartz windows. The magnet was funded by a NSF IMR Grant and is now operational. For more information on this work, see: Tyson, et at., Phys. Rev. B, 70, 024410 (2004).

The magnet setup at X19A. It is mounted on an xyz table, which can be motor-controlled for ease of alignment. Samples are loaded from the top on a vertical rod into the sample space and are cooled by helium vapor or liquid from the magnet reservoir.



X-Ray Ring Long-Range Schedule

May 2005

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29 0000 Cond.	**30 Lab Holiday** 0000 Cond.	**31** 0000 Beam Observation				

June 2005

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July 2005

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August 2005

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VUV-IR Ring Long-Range Schedule

May 2005

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June 2005

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July 2005

Sun	Mon	Tue	Wed	Thu	Fri	Sat
					1 0000 Ops. 1900 Holiday	**2 Lab Holiday** No Beam
3 Lab Holiday No Beam	**4 Lab Holiday** No Beam	**5 Lab Holiday** No Beam	**6** 0000 Maint.	**7** 0000 Maint.	**8** 0000 Cond.	**9** 0000 Cond.
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August 2005

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The Structure of Ba@C_{74}

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For the first time, the structure of a monometallofullerene has been analyzed using single crystal synchrotron diffraction on microcrystals of Ba@C_{74}·Co(OEP)·2C_6H_6 (where Co(OEP) is cobalt(II)-octaethylporphyrin) at 100 K. This monometallofullerene exhibits a high degree of localization of its endohedral metal ion, with just two split positions for barium and two orientations for the C_{74} cage. The crystal structure consists of complex units (Ba@C_{74})[Co(OEP)]$_2$(Ba@C_{74}) arranged in a distorted, primitive hexagonal packing. Despite the disorder still present, we have derived a consistent and conclusive structure model for the title compound by employing a combination of x-ray diffraction, x-ray absorption near-edge structure (XANES) spectroscopy, and quantum chemical calculations.


Dr. Andreas Reich


Dr. Martin Panthöfer


Dr. Hartwig Modrow


Dr. Ulrich Wedig


Prof. Martin Jansen

Since the discovery of fullerenes, information about the molecular and electronic structure of this new family of carbon allotropes, which include "endohedral" metallofullerenes (those with metal atoms inside the fullerene cage) and fullerene compounds, has been essential for understanding their physical and chemical properties. To acquire such information, the availability of precise crystal structure data is a crucial prerequisite.

In ongoing research efforts, we have developed a method that allows a high-yield synthesis of small and mid-sized endohedral fullerenes consisting of divalent metals that follow M@C_m (where m = 60, 70, 72, 74, 76; M = Ca, Sr, Ba, Eu). In this method, we inductively heat graphite and the corresponding metal inside a radiofrequency field to temperatures of up to 3000 K (**Figure 1**), and then isolate individual species from the raw soot extracts using multi-step high-performance liquid chromatography (HPLC).

By employing micro-crystal synchrotron diffraction techniques, computational chemistry, and XANES spectroscopy in a synergetic manner, we were able to determine the structure of Ba@C_{74} as a co-crystallizate with Co-octaethylporphyrin (Co(OEP)) and C_6H_6 (benzene).

The crystal structure of Ba@C_{74}·Co(OEP)·2C_6H_6 consists of complex units (Ba@C_{74})[Co(OEP)]$_2$(Ba@C_{74}) exhibiting a back-to-back orientation of two Co(OEP) molecules, each coordinating one Ba@C_{74} molecule (**Figure 2**). The overall structure may be regarded as a distorted, primitive hexagonal packing of these complex units. Yet, the fullerene substructure is disordered, with two orientations for the C_{74} cage and two positions for the barium atom. Thus, four different barium-to-C_{74} coordination schemes have to be discussed. Out of those, two are similar to those found from the results of the quantum-chemical investigations. Yet, the shortest Ba-C distances do not correspond to the central 6:6 bond of a pyracylene unit located at one of the three pockets of the cloverleaf-shaped C_{74} molecule, but to its vicinity.


***Figure 1**. The radio-frequency furnace for endohedral fullerene synthesis in action.*

As stated above, computational investigations on Ba@C_{74} show that the local minimum structure of Ba@C_{74} corresponds to a 3-fold degenerate arrangement with barium located in one of the three pockets of C_{74}, coordinating to the central 6:6 pyracylene bond. Remarkably, the molecular structure of the neutral C_{74} cage in Ba@C_{74} differs only slightly from the molecular structure of a C_{74}^{2-} dianion (both determined using the density-functional theory in local-density approximation).

Those differences are highly localized in the central 6:6 bond of the pyracylene units.

This discrepancy between the results of the experimental and the computational investigations is clearly due to the intermolecular interactions present in the co-crystallizate. On one hand, those Co(OEP)-Ba@C_{74} configurations that result in a large contact surface between the two molecules allow attractive π-π and dispersion interactions. On the other hand, configurations where the pyracylene unit at the pocket of Ba@C_{74} is pointed towards the Co-atom of the Co(OEP) molecule allow stabilization via multipole-multipole interactions. The competition between these two different intermolecular interactions triggers the orientational disorder of the C_{74} cage. Furthermore, molecular dynamics simulations reveal a nearly flat potential hypersurface around the local minima positions within the pocket of the cloverleaf-shaped molecule. This suggests an easy displacement of the Ba atom near a minimum that is produced by a direct interaction between the Ba^{2+} cation and the Co(OEP) molecule. Thus, the positional disorder of the barium atom is a consequence of the orientational disorder of the C_{74} cage, which is due to the competition of π-π and electrostatic interactions.

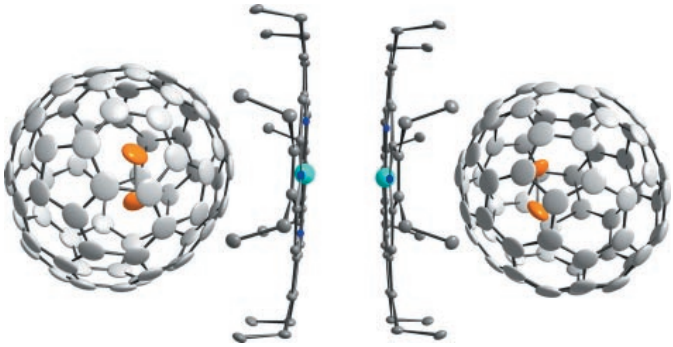


***Figure 2**. A (Ba@C_{74})[Co(OEP)]$_2$(Ba@C_{74}) unit in Ba@C_{74}·Co(OEP)·2C_6H_6 (for clarity, only one fullerene orientation is given).*

For more details of this work see: A. Reich, M. Panthöfer, H. Modrow, U. Wedig, M. Jansen, "The Structure of Ba@C_{74}," J. Am. Chem. Soc., 126 (44), 14428-14434 (2004).

AWARDS

NSLS Engineer John Skaritka Wins BNL's Engineering Award

Liz Seubert, BNL Media & Communications Office

At the BNL Employee Recognition Award Ceremony held on January 26, 2005 NSLS engineer John Skaritka was presented a FY2005 Engineering Award by BNL's Deputy Director for Operations, Michael Bebon. The award, consisting of a plaque and $5,000, was also presented to BNL employees Ove Dyling, Joseph Harder, and Alan Raphael.

The award recognizes distinguished contributions to BNL's engineering and computing objectives over one or more years. Contributions may be in any engineering or computing discipline. Nominees are evaluated on the exceptional nature and level of difficulty of the contributions as well as their benefit to the Lab.

John Skaritka was cited for a body of work that contains seminal as well as sustained contributions. His many achievements speak collectively to outstanding breadth, creativity, drive, and dedication in support of BNL missions.

John Skaritka

Skaritka was the sole mechanical engineer for BNL's Accelerator Test Facility (ATF) for many years, making key contributions to the design of elements of the accelerator and experiments that were essential to the success of those projects. He contributed to the design of ATF Gun III and Gun IV, regarded now as standard in the world and running at many other facilities.

He was also the mechanical engineer in charge of coordinating all mechanical design, fabrication, and installation activities at the Source Development Laboratory, resulting in a state-of-the art facility that produced both a self-amplified spontaneous-emission free-electron laser and a high-gain harmonic generation free-electron laser.

Skaritka is also known for his considerable talent in supporting the NSLS User Science programs, recently, for example, in the construction of a unique instrument pivotal in research on three-dimensional strain mapping to study crack propagation and fatigue failure in alloys.

What's New at User Administration

Mary Anne Corwin, NSLS User Administrator

Paperless Office

A milestone was achieved by the fiscal year's end in converting User Administration into a paperless office. As time and resources permitted over the last three years, existing records were scanned; new records are generated electronically. This accomplishment resulted in an $8K budget savings and eliminated the need for 280 cubic feet of office space. We exceeded DOE's and BNL's goals in reducing consumption and waste and are at the forefront in electronic records retention, significantly facilitating audits and records retrieval.

BNL Site Access

Site access policies require that users produce valid BNL identification badges or have active or pending appointments. A badge scanning system notifies the officer at the gate of problems with a user's appointment or visa status. These users are informed to check in at User Administration. Users are reminded that they cannot begin work or access the experimental floor until the user has checked in and fulfilled the necessary requirements.

Check-in/Check-Out System

To facilitate site access, all users are reminded to complete BNL's check-in/check-out online form in advance at *https://fsd84.bis.bnl.gov/guest/chkinout.login.asp*. User Administration generates daily reports to verify users have arrived, have valid appointments, are in visa status, and to enter departure dates. The out system will be upgraded soon to notify users of expiring appointments and visas.

Visas for Foreign Nationals

As a convenience, users are issued two-year appointments, sometimes extending beyond their visa expiration date. A new visa must be presented each time the documents we have on file expire. Visas vary from 90 days to several years. Users with short-term visas should schedule beam time during the work week to ensure they will be permitted to work on arrival. Several users had to return home to retrieve their documents before starting their experiment. Additionally, users with B2 and WT visas are not permitted to perform experiments and must return to the port of entry within 24 hours to obtain corrected documents.

Instances of non-compliance have resulted from users who were out of visa status and began their experiments after being informed by BNL officers to check in at User Administration but failed to do so. Please do not jeopardize your appointment. We urge all foreign national users to bring valid passports, visas, and supporting documents during each visit.

Experimental Floor Access

We found instances of safety non-compliance where users accessed the experimental floor with expired or no training. To eliminate these problems, as well as non-compliances by foreign nationals, User Administration now provides "timed-access" to expire with the first expiration of training, ID badge, passport, or visa status dates. Modifications to the PASS system were made to ensure that experimenters are listed on safety approval forms and are in compliance. And, the laboratory's training record database (BTMS) now generates automatic emails to users whose training has expired.

Benefits to Compliance

With limited resources, we're very grateful to our users who help us maintain compliance with DOE directives. By eliminating non-compliances, we can focus more on user-related quality-of-life issues. We encourage our users to contact User Administration at (631) 344-USER (or nslsuser@bnl.gov) with any additional recommendations to eliminate non-compliances or with any questions.

Weekly NSLS Activities

For more information about the following activities visit: http://www.nsls.bnl.gov/newsroom/events/weekly_meetings.htm.

Tuesday

Bi-Monthly Symposia: 10:30 to 11:30 a.m., Seminar Room. See URL below for Symposium calendar: *http://www.nsls.bnl.gov/newsroom/events/seminars.htm*

Wednesday

Joint VUV and X-Ray Users' Meeting: 11:30 a.m., Seminar Room.

Coffee for Users and Staff: 3:30 p.m., NSLS Lobby.

Thursday

Student/Postdoc Pizza Get-Together: Every other Thursday, 1:30 p.m, Room 1-109 on the UV floor (corner kitchen).

Friday

Friday Lunch Seminars: 12:00 to 1:00 p.m., Seminar Room.

NSLS Accelerator Complex Update

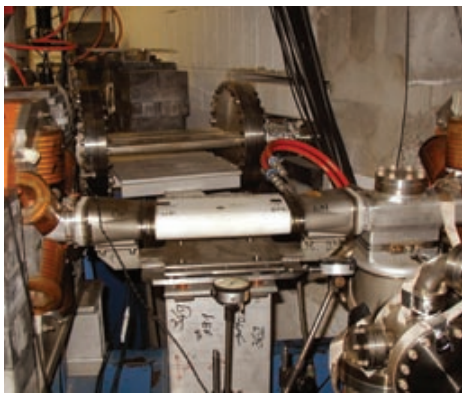
Erik Johnson, Associate Chair for Operations and Engineering

As of March 1st, reliability of both the VUV and x-ray rings exceeded 95% for fiscal year 2005, meeting our department goal for user operations. Our preventative maintenance program is an important contributor to this success. The recently completed winter shutdown included many routine maintenance items, as well as equipment safety upgrades and a few major installations. One major task was the replacement of an injection ceramic for the XIFB1 bump on the x-ray ring that had begun to leak over the summer. Since this work required venting superperiod 8, the water-cooled 'speedbump' downstream of X1 was also removed. The water-cooling had been removed some time ago due to a leak, and with the advent of the active interlock system it was no longer required.

The return to operations was uneventful, although we experienced some orbit distortions that required corrections, which impacted user operations. To avoid this problem in future, we have scheduled two days at the end of the May shutdown for beam observations on the x-ray ring. This time will be used to make any corrections that are necessary before scheduled user operations. I would like to encourage all of the x-ray beamlines to be prepared to take advantage of this time so that we can minimize disruption of user operations once the scheduling cycle starts.

The work planned for the May shutdown includes upgrading the UV RF temperature control system, maintenance and rebuild activities for the X-17 cryogenics plant, general preventative maintenance, and continuing equipment safety upgrades. There will also be maintenance on the electrical substations that will shut off the entire building. The substation work is scheduled for Saturday, May 14, with May 21 as a rain date.

Finally, thanks again to all who provided input for the Summer 2005 schedule. Working around the holidays resulted in a somewhat eccentric schedule but it met most of the requests and actually provides about the same user time as comparable schedules in the past. The Fall 2005 schedule will be finalized in May, so if there are any special scheduling considerations please let me know by April 2005.



The XIFB1 ceramic shown here was replaced in the December 2004 shutdown. It is one of four ceramic chambers for injection on the x-ray ring. The BXISH ceramic was replaced in May of 2004.

SBU/BNL Van Route Schedule

Monday - Friday (except holidays)

Pick Up Time	Pick Up Location	Drop Off Time	Drop Off Location
8:30 am	SBU-SAC Loop	9:15 am	BNL-Berkner Hall
9:30 am	BNL-Berkner Hall	10:15 am	SBU-SAC Loop
12:00 pm	SBU-SAC Loop	12:45 pm	BNL-Berkner Hall
1:00 pm	BNL-Berkner Hall	1:45 pm	SBU-SAC Loop
4:30 pm	SBU-SAC Loop	5:15 pm	BNL-Berkner Hall
5:30 pm	BNL-Berkner Hall	6:15 pm	SBU-SAC Loop

If you have any questions or concerns regarding the van, please contact Elyce Acierno at 631-632-4360 or Elyce.Acierno@stonybrook.edu. For the most up-to-date schedule, see: http://www.bnl.gov/staffservices/Transportation/transportation.asp.

Electrical Safety at the NSLS: What is NFPA 70E?

Andrew Ackerman, NSLS Safety Officer

Electrical safety remains an important priority at the NSLS. We want you to know about this changing program and we ask that you help us manage the risks presented by electric power distribution and use at the facility.

Our colleagues at the Department of Energy (DOE) have mandated that we improve our electrical safety program, but that is really only part of our motivation, as we have long seen this need and we welcome the increased attention. We consider risk of electric shock or fire to be among the more significant concerns that we manage, and part of our safety program is to make sure that our user community is informed and prepared to meet electrical safety requirements.

As a user, you must know the electrical safety precautions needed for the tasks that you perform or plan and we ask that you disseminate electric safety information to all of our other users. Everyone working on the experiment floor or sending someone to work at one of our beamlines must help us with this effort. These are real risks that, if not respected, could have severe consequences.

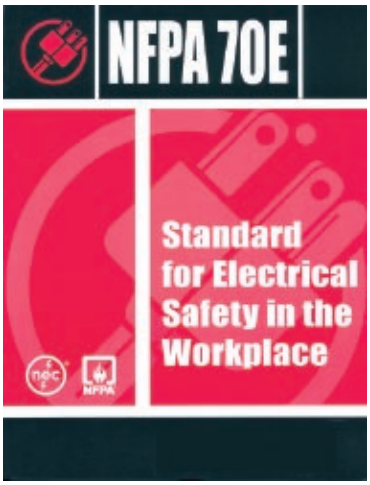
NFPA 70E is the reference you should be hearing about. It is intended to provide a concise set of workplace electrical safety requirements to enhance existing OSHA requirements and also remain consistent with the National Electric Code (NEC). The first edition was published in 1979. The new 2004 edition is the seventh revision and is well organized into four chapters: work practices, maintenance, special equipment, and installation.

The work practices chapter provides some general safety requirements, requirements for lock out/tag out (LOTO), and specific requirements for what is defined as working on or near energized components. This is the chapter that you need to know about if you service, repair, or troubleshoot range B electric-powered equipment at the NSLS.

Chapter 1 of 70E contains requirements for conducting both shock and flash protection hazard analyses to establish approach boundary distances and determine needed controls. Users who must LOTO range B electrical equipment or who must work on range B energized circuits must cross those boundaries and so must be protected from both risks. You'll need a permit, personal protective equipment, and training. We are working to keep this process simple, but the 70E requirements are restrictive. You can expect to be wearing voltage-rated gloves, eye protection, fire-rated garments, and a hard hat for zero-energy verification or work on energized circuits in range B. You can also expect not to measure or troubleshoot any energized circuits with specifications that exceed range B. You will need help from a BNL electrician for that.

Chapter 4 of 70E covers the assembly and installation of equipment that mostly applies to facility-level work, but there are requirements that could apply to the assembly of equipment components used for experiments and beamlines. If you build an electric device that uses range B power, you must meet requirements for enclosure, insulation, wiring, and grounding. The requirements are not complicated, but meeting them means planning and having the proper components and tools.

So, if none of this is familiar to you, you do not bring any self-assembled equipment to the NSLS, and you do not modify powered systems, you need not be concerned with these terms and acronyms. But if you do work with this equipment, these requirements will impact your experiment planning and will require some effort to keep your work safe. Scientists who work with electric power must know and plan for the safety requirements that apply to their experiments and, of course, are encouraged to come for help when needed.



The NSLS Newsletter is printed on paper containing at least 25 percent recycled materials, with 10 percent post-consumer waste.

Upcoming Workshops and Seminars

Strain Mapping in Engineering Materials with High-Energy Synchrotron X-Rays

April 18-19, 2005

This workshop brings together key members of the synchrotron community and experts in engineering materials science to discuss and explore the current and potential applications of high-energy x-ray strain mapping to engineering problems, and to catalyze new interactions between these fields. The workshop will assess the user base for beamline X17, identify potential funding sources, and determine the viability of additional dedicated experimental hutch space on X17. Invitees will be asked to propose experiments that define what apparatus and conditions would be conducive to their research. It will also provide a forum to discuss future strain mapping research and its potential use at the proposed NSLS-II. Additional information on the workshop is available at: *http://www.nsls.bnl.gov/newsroom/events/workshops/strain/*.

The X6A Workbench: Advanced Structural Biology Tools

April 26-29 and July 12-15, 2005

The NIGMS facility at the NSLS is offering comprehensive hands-on training in synchrotron data collection and analysis for biophysicists, biochemists, and molecular biologists. The goal is to give participants insight into structural biology methods. Applications can be sent anytime. Four experimenters will be selected bi-monthly and invited to participate in this four-day program. The program will concentrate on the development of experimental skills. Introductory lectures will be presented by local experts. Participants can bring their own samples for the experiments but samples will be provided for training. The X6A workbench is regularly offered throughout the year. The next two workshops are scheduled for April 26-29 and July 12-15, 2005. More information, including registration, can be found at: *http://protein.nsls.bnl.gov/news/workbench.php*.

2005 NSLS Annual Users' Meeting

May 23-25, 2005

The NSLS Annual Users' Meeting is a forum for reporting new research results and advances in experimental capabilities that utilize synchrotron light, hosted and sponsored by the NSLS Users' Association. The meeting brings together scientists from many disciplines to share their recent accomplishments at the NSLS and visions of the future, through workshops, invited talks, the poster session, exhibits, and informal interactions. Infrequent and new users are especially encouraged to attend. The meeting and workshops are supported by registration fees paid by the participants. Social events, lunches, coffee breaks, and associated expenses are supported primarily by our vendors and sponsors, and in part by Brookhaven National Laboratory's Light Sources Directorate. More information, including online registration, can be found on the web at: *http://www.nsls.bnl.gov/users/meeting/*.

Crystallization: Focus on Optimization Techniques for Soluble and Membrane Proteins

June 6-8, 2005

This workshop is designed to provide participants with hands-on experience using a variety of crystal-growth methods for obtaining high-quality crystals. Introductory lectures will precede each of the eight practical sessions and time has been allotted for discussions and informal meetings. On the last day, a special session on cryogenic protection and crystal quality will be held at beamline X6A. There is no selection criteria for participants, and the deadline for application is May 1, 2005. The course is sponsored by Nextal Biotechnologies, Hampton Research, deCode Genetics, Fluidigm Corporation, Jena Bioscience, Molecular Dimensions, Precision Detectors, and GE-Healthcare. The application form and other information about the workshop are posted online at: *http://www.nsls.bnl.gov/newsroom/events/workshops/crys/*.

BioCD-2005: Short Course in Circular Dichroism Spectroscopy of Proteins & Nucleic Acids

June 20-25, 2005

The purpose of this workshop is to train researchers in the use of circular dichroism (CD) spectroscopy for characterizing proteins and nucleic acids in solution. Lectures will include principles of CD and its application to the analysis of the structure of globular proteins, membrane-bound proteins, and nucleic acids. Laboratory sessions will focus on sample preparation, calibration, and data collection using conventional and synchrotron-source spectrometers, web resources for analysis of protein structures, and time-resolved CD. The workshop, limited to approximately 12 participants, is intended for new users and young graduate, postdoctoral, and research scientists. The application deadline is May 1, 2005. The workshop is sponsored by the Biology and NSLS departments at Brookhaven National Laboratory, which are funded by the U.S. Department of Energy's Office of Science. More information on the course and registration can be found at: *http://www.nsls.bnl.gov/newsroom/events/workshops/biocd/*.

NSLS Information and Outreach Office
Brookhaven National Laboratory
NSLS Building 725B
P.O. Box 5000
Upton, NY 11973-5000

Call for NSLS General User Proposals

For Beam Time in Cycle	Deadline
September - December 2005	Tuesday, May 31, 2005

General User Proposal and Beam Time Request Forms with instructions can be found at:
http://www.nsls.bnl.gov/users/usersguide/experiments.htm
Proprietary Proposal Forms with instructions can be found at:
http://www.nsls.bnl.gov/users/usersguide/experiments_proprietary.htm

Safety Approval Forms

Safety Approval Forms (SAFs) are required for every experiment. Your SAF must be submitted online **at least one week before** your scheduled beam time. To submit, go to:

https://pass.nsls.bnl.gov/

NSLS User Administration Office

User Information, Registration, and Training:
Phone: (631) 344-USER Fax: (631) 344-7206

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