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ALS Users' Meeting and Workshops

2010 ALS Users' Meeting—Innovative Firsts and Spectacular Science

For the nearly 400 attendees, the 2010 ALS Users' Meeting was a smashing success. In his opening remarks, Users' Executive Committee (UEC) Chair David Osborn thanked meeting co-chairs Hendrik Bluhm and Brandy Toner for what was to be an enjoyable and stimulating conference and a year of innovation with the first Student Poster Slam and ALS Photography Competition.

ALS Director Roger Falcone opened the meeting by announcing, "The ALS is very healthy!" This year the ALS welcomed new staff, built new beamlines, increased proposals and remote usership, and received an R&D 100 award for APPELS, its ambient-pressure

research instrument. "The ALS accelerator is at the forefront of performance globally," Falcone said. "The stimulus money received in FY09 helped to launch our renewal," which is well underway.

Dr. Harriet Kung, Department of Energy (DOE) Associate Director of Science for Basic Energy Sciences, focused on the need to discover new, earth-abundant materials using computational, chemical, and materials sciences. Kung praised the new User Support Building (USB) as "a success in project management: heartening, early, and under budget. A true highlight." Michael Lubell, Director of Public Affairs for the American Physical



Figure 1: ALS Director Roger Falcone; Congressman Vern Ehlers (R-MI); State Assemblywoman Nancy Skinner; Bruce Darling, the UC Lab Management Director for Lawrence Berkeley, Lawrence Livermore, and Los Alamos National Laboratories; Dr. Harriet Kung; State Senator Loni Hancock; and ALS UEC Chair David Osborn.

Society, followed Kung, speaking about the prospects for American science. Congressman Vern Ehlers (R-MI) pondered how to increase awareness amongst politicians and the public of science and its impacts on everyday life. "Energy is the most basic natural resource because without it we cannot use other natural resources," Ehlers said. Donald DePaolo (Earth Sciences Division, Berkeley Lab) rounded out the morning session discussing research challenges in earth and environmental science.

The USB was formally opened in a well-attended ribbon-cutting ceremony, where it received rave reviews as Berkeley Lab's newest building. The USB is "highly functional and stunningly beautiful," said Bruce Darling, University of California (UC) Lab Management Director. "It really epitomizes DOE goals for growth," Kung added. UEC Chair David Osborn thanked ALS staff during the ceremony: "On behalf of users, I'd like to convey sincere appreciation to Roger (Falcone), Steve (Rossi), and other teams. You listened to users."

In the afternoon, Steve Rossi, Dave Robin, and Jim Floyd gave updates on the

USB, operations, and safety, respectively. Zahid Hussain updated users on MERLIN, ARPES' new VLS spectrometer that is unique worldwide, and the Berkeley Synchrotron Infrared Structural Biology Program. Patrick Naulleau of the Center for X-Ray Optics (CXRO) gave an overview of their research programs and plans for new 8-nm-resolution lithography and microscope tools. A lively open forum brought discussion on what to do with unscheduled beam time, and feedback on the Guest House. Users also decided by a vote that they prefer the beam to be off during the meeting.

The Lab's main auditorium was packed to hear invited science highlight talks. Aaron Bostwick showcased his study of graphene using photoemission. George Cody pondered the composition of chondrites and the existence of wet comets. Bill McCurdy gave a preview of soft X-ray science over the next 10 years, stressing the importance of understanding artificial photosynthesis and variable charge-transfer dynamics in molecules and complexes.

The Student Poster Slam was a giant success: 24 students each spoke for 50 seconds about their posters. Nearly all stayed within their allotted time, and the audience was enthralled! Graduate students from Switzerland, Hungary, Mexico, and China made up most of the group, along with five students from the University of Saskatchewan and one UC Berkeley undergraduate.

The Thursday morning session began with a presentation by Hoi-Ying Holman, awarded the David A. Shirley Award for Outstanding Scientific Achievement at the ALS for her "pioneering study of living cells and their response to environmental stimuli using synchrotron-based FTIR spectromicroscopy." Her talk, "Synchrotron Infrared Spectroscopy and the Gulf of Mexico Deep-Sea Oil Plume," detailed alternate ways to think about microbial community composition and function in environments like the Gulf of Mexico. This work was particularly relevant following the blowout of the Macondo Well (better known as the Deepwater Horizon oil rig explosion), where the escaping oil's biological effects and expected fate are unknown

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due partly to the extreme depth and magnitude of this event. By using FTIR spectromicroscopy, Holman demonstrated molecular measurements of in-situ microbial processes that revealed how indigenous deep-sea microbes have the potential for bioremediation of oil hydrocarbons in the deep-water oil plume in the Gulf of Mexico.

Weilun Chao, representing the team (Erik Anderson, Weilun Chao, Peter Fischer, Tolek Tyliczszak, David Kilcoyne, and Tony Warwick) that won the Klaus Halbach Award for Innovative Instrumentation at the ALS for "hitting the 10-nm resolution milestone with soft-X-ray microscopy," described a new overlay nanofabrication technique for narrower outer-zone creation that aided in the achievement of 12-nm outer-zone lines and 10-nm resolution for both full-field and scanning microscopes—world records in X-ray microscopy.

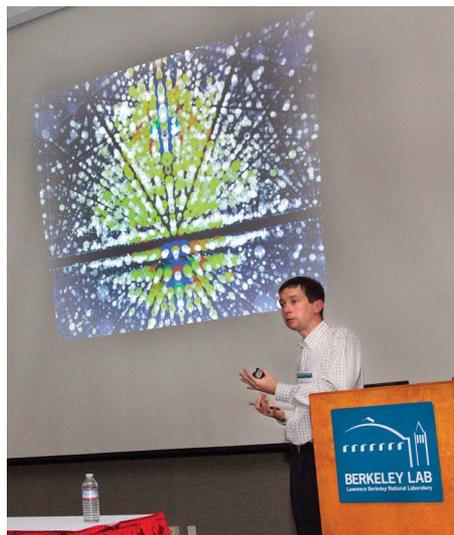


Figure 2: Henry Chapman shares diffractive imaging results from experiments at various light sources during an evening lecture honoring former ALS Acting Director Janos Kirz.

MEETING REPORTS

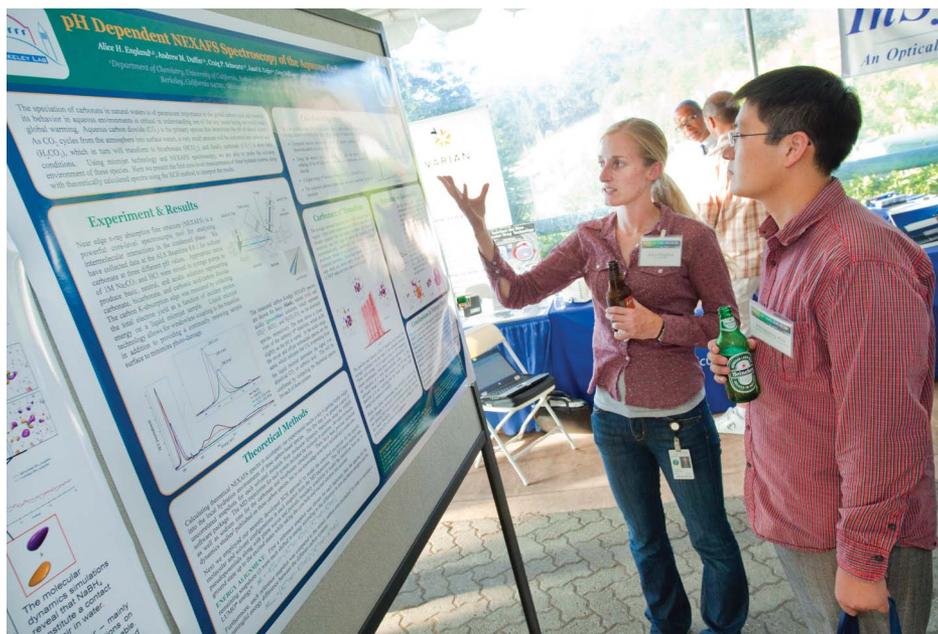


Figure 3: Alice H. England answers questions about her poster "pH dependent NEXAFS Spectroscopy of the Aqueous Carbonate System" during a poster session.

The Student Poster Award winner was Robert Green, University of Saskatchewan. His engaging presentation highlighted the doping of semiconductors to create dilute magnetic semiconductors and subsequent measurement of the energy dependence of photon absorption and decay using XAS and RIXS, respectively.

The awards banquet was so well attended the ALS patio had standing room only. Award-ees were lauded for their contributions to the ALS; participants then honored former ALS Acting Director Janos Kirz with an evening lecture on the history of diffractive imaging by his former student, Henry Chapman.

Workshops preceded the awards banquet Thursday and continued Friday. Selected workshop reports are presented below. More detailed information can be found at <http://www-als.lbl.gov/index.php/user-information/users-meeting.html>. ■

SHAUNA KANEL
Advanced Light Source

ALS Users' Meeting and Workshops

Infrared Spectromicroscopy Workshop: The Berkeley Synchrotron Infrared Structural Biology (BSISB) Program

The Berkeley Synchrotron Infrared Structural Biology (BSISB) program held a workshop to familiarize potential users of the new ALS infrared Beamline 5.4 with the wide variety of science that can be performed using the novel tools available at this facility. BSISB is directed by Hoi-Ying Holman and is funded by the Office of Biological and Environmental Research within the Department of Energy. The workshop spanned two days, October 14 and 15, 2010.

The first day of the workshop brought together scientists from different areas including biofuel, carbon sequestration,

low-dose radiation, and medicine to discuss various scientific efforts and the infrared tools required to enable them. The speakers and their topics are posted online at <http://infrared.als.lbl.gov/content/structuralbiology/workshop>.

The second day of the workshop, which was jointly held with Thermo-Fisher Scientific, provided tutorials and hands-on opportunities on the FTIR and Raman systems at Beamline 5.4. Hoi-Ying Holman concluded the workshop with a demonstration of how to successfully prepare and measure living cellular systems. The discussion focused on



Jessica Dittmar (Stanford University) measures a sample with FTIR spectroscopy at the new ALS Beamline 5.4.

methods to achieve and maintain enough water in the culture media to support cell function while preventing the water from obscuring the infrared signals of interest.

We feel the workshop was a great success and are all looking forward to the science that will be done with the new BSISB program's capabilities at Beamline 5.4 at the ALS.■

MICHAEL MARTIN AND HANS BECHTEL
Advanced Light Source

PETER NICO AND HOI-YING HOLMAN
Earth Sciences Division, Berkeley Lab

ALS Users' Meeting and Workshops

Defects in Inorganic Solids and their Relation to Electronic Properties

This workshop focused on the role of imperfections in inorganic materials and their relation to electronic transport properties. The workshop covered investigations of materials with relevance to electrochemical energy storage and solar energy conversion systems, solid-liquid interfaces, computational defect modeling, and the experimental assessment of the electronic structure of materials with resonant inelastic X-ray scattering.

Matthew Marcus (ALS) gave a short keynote presentation to set a unifying theme. The idea is that X-ray techniques allow defect studies to enter new regimes in which defect concentrations are large, samples are not single crystals, the host lattice may be highly perturbed by defects, and *in situ* or

operando conditions may be required. Bonna Newman (MIT) showed how ultrafast optical laser processing can force silicon to tolerate extremely high defect densities by hyperdoping with chalcogens. The assessment of the electronic structure of such hyperdoped silicon was then detailed by Lothar Weinhardt (Universität Würzburg). Su-Huai Wei (NREL) explained the theoretical origin of the doping difficulty in wide-band-gap semiconductors and discussed strategies for how to overcome said limitations. Tony Van Buuren (LLNL) presented a spectro-electrochemical, *in situ* reaction cell suitable for the soft X-ray range that had been used for the characterization of novel lithium-battery electrode materials during charging and discharging. Glenn Waychunas (Environmental

Energy Technologies Division, Berkeley Lab) explained how mineral surfaces in contact with water typically differ from clean in-vacuum surfaces. It was also explained how the water at the interface differs from the bulk, and how the zone of highly ordered water at the interface may be important in nanoparticle aggregation and certain types of geochemically relevant reactions.■

MATTHEW MARCUS AND JINGHUA GUO
Advanced Light Source

ARTUR BRAUN
Empa, Switzerland

CLEMENS HESKE
University of Nevada, Las Vegas

ALS Users' Meeting and Workshops

Workshop on Spin-Resolved Photoemission at the Advanced Light Source

The addition of spin resolution to photoemission was an important step in experimental studies of band structure in magnetic

materials. Recently, demand for spin resolution has surged due to the emergence of interesting new materials, such as topological

insulators with surface states possessing unique spin textures, materials with the Rashba split spin-polarized surface states, and

materials relevant to spintronics. Luckily, instrumentation for spin-resolved measurements has been steadily improving over the same period, enabling many measurements that were impossible just a decade ago.

To ensure that a broader user community has access to spin-resolved photoemission instrumentation, the Scientific Support Group at the ALS has decided to supplement its ARPES facility at Beamline 12.0.1 with a permanent station for spin-resolved ARPES, available to users during multibunch operation. If work proceeds according to schedule, this facility will be commissioned by the end of 2011.

A two-day workshop during the 2010 ALS Users' Meeting brought together experts in spin-resolved photoemission and current users of ARPES facilities at the ALS who are planning to perform spin-resolved

photoemission experiments in the future. The workshop included 17 invited presentations by speakers from the United States and Europe and was one of the most well-attended workshops at the meeting. The talks encompassed instrumentation developments, recent results, future studies, and theoretical aspects of spin-resolved photoemission applied to strongly correlated materials. The speakers, their topics, and their abstracts and presentations (when available) are posted online at http://physics.berkeley.edu/research/lanzara/Spin%20Workshop/Spin_pageA.html.

Invited talks were complemented by lively discussions and tours of the ALS beamlines and the photoemission laboratory maintained by the group of A. Lanzara. The participants of this first-ever meeting dedicated specifically to spin-resolved photoemission univocally praised



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the dedication of the ALS to establishing a facility for spin-resolved ARPES.■

ALEXEI FEDOROV
Advanced Light Source

CHRIS JOZWIAK
*Advanced Light Source and University of
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ALESSANDRA LANZARA
University of California, Berkeley



ALS Workshop on Spin-Resolved Photoemission: participants freed from discussions posed for a picture taken just before the last session of the workshop.

ALS Users' Meeting and Workshops

TIPS: Theory Institute for Photon Science



John Rehr (University of Washington) explains his view of "Tools for a Next Generation X-ray Beamline: XAS, XES, and RIXS."

The experimental requirements for addressing our scientific grand challenges will require the development of future light sources based on free-electron lasers as well as the continuing development of more precise and flexible instruments that would propel us beyond

observation science to control science. However, these current and future light sources will fall well short of their potential without a significant dedicated theoretical effort.

This workshop was held as an important step toward the development of a Theory Institute for Photon Science (TIPS). This institute intends to provide vigorous theoretical support in meeting the five DOE Grand Challenges. It will stimulate the development of theoretical methods for the interpretation of experimental data and for computing the measurable properties of complex systems. More broadly, the primary mission of TIPS will be to initiate strong interactions between experimentalists and theorists that will enhance not only the productivity of users but also the process of scientific discovery.

The workshop brought together over 50 internationally recognized theoretical experts with a wide range of interests in complex/

correlated electronic materials, nanomaterials, and interfacial phenomena. The speakers, their topics, and their abstracts (when available) are posted online at http://bl7-wiki.als.lbl.gov/mediawiki/index.php/TIPS_Workshop.

A mix of permanent faculty/staff collaborators, visitors, postdoctoral fellows, and graduate students will enable TIPS to create an environment of strong scientific collaborations. TIPS will attract the brightest theorists in diverse academic disciplines (chemistry, materials science, and physics) to work on photon science through innovative collaborations. ■

JINGHUA GUO AND ZAHID HUSSAIN
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ARUN BANSIL
Department of Physics, Northeastern University

ALS Users' Meeting and Workshops

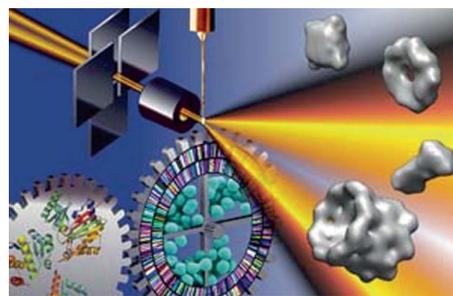
Practical Course on SAXS from Biological Material

The SAXS technique has been rediscovered in recent years by an increasing number of structural biologists to complement high-resolution structural studies by crystallography, EM, and NMR. The SIBYLS team at ALS Beamline 12.3.1 hosted a workshop emphasizing experimental aspects of noncrystalline diffraction techniques in biology. Forty scientists participated in the workshop, which provided hands-on training in experimental techniques and software tutorial sessions. One day shift of beam time was allocated during the workshop for short data-collection runs. In this practical session, workshop participants got hands-on experience with SAXS measurements. At the end of the day, participating students were able

to analyze their own experimental data collected automatically in high-throughput mode.

The success of this SAXS workshop is underscored by testimonials from workshop participants with all levels of SAXS experience, including Artem Lyubimov's comment, "I learned more about SAXS in two days than in the last two years." Min Guo noted, "Hope you will soon see several papers showing up from our group." Hari Kamadurai stated, "We managed to get some useful data from the workshop and I am quite excited about it." ■

MICHAL HAMMEL, GREGORY HURA,
AND SCOTT CLASSEN
Physical Biosciences Division, Berkeley Lab



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

ALS Users' Meeting and Workshops

Workshop on Soft X-ray Spectroscopy for Electrochemical Applications/Batteries

The urgent need for high-performance, robust, and safe electrochemical devices and the scientific challenges in the path to achieving these goals were the motivation for bringing together experts in the areas of material synthesis, characterization, and simulation as applied to electrochemical devices such as batteries and fuel cells to attend this workshop. The workshop in particular addressed how synchrotron-based techniques, especially soft X-ray spectroscopy, can be used in the control feedback loop to improve electrochemical device design. During the workshop, the invited speakers and participants discussed current progress in electrochemical applications,

scientific opportunities for using soft X-ray spectroscopy, and necessary technical improvements. The consequences of increased user demand on existing beamlines and ways to expand the availability of time were also considered. About 45 participants attended this workshop. The speakers, their topics, and their abstracts are posted online at <https://sites.google.com/a/lbl.gov/2010-electrochemistry-als-workshop/>.

Potential collaborations among the participants were also initiated through the discussion. The large number of attendees from different research fields demonstrated that a robust and vibrant interdisciplinary community

has formed and is growing rapidly. All participants of the workshop agreed that there is an urgent need for in situ X-ray spectroscopy facilities, which are crucial for developing the next generation of energy conversion and storage devices, a key component to a clean and secure energy future. ■

HENDRIK BLUHM

Chemical Sciences Division, Berkeley Lab

ZAHID HUSSAIN, JINGHUA GUO,

ZHI LIU, AND WANLI YANG

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