MEETING PROGRAM

Sponsored by the NSLS-II and CFN
Users’ Executive Committee
Welcome to the 2017 NSLS-II & CFN Users’ Meeting!

We are very pleased that you have joined us for the 2017 National Synchrotron Light Source II (NSLS-II) and Center for Functional Nanomaterials (CFN) Users’ Meeting.

This year, the theme of our meeting is “Making and Measuring in 4-Dimensions” as we focus on the exciting new prospects of NSLS-II, and the continuing excellence of CFN. The program includes invited talks, workshops, a poster session, and exhibits highlighting new technology and instrumentation - all offering opportunities to learn about the latest developments in synchrotron and nanoscience experimentation and how they might impact your research.

The Plenary session will be held on Tuesday. The key note speaker will be Teri W. Odom, Charles E. and Emma H. Morrison Professor; Associate Chair of the Department of Chemistry, Northwestern University along with invited speakers, Christophe Detavernier, Prof. Ghent University, Belgium, and Mark Sutton, Prof. McGill University, Canada., An update on the NSLS-II Strategic Plan from Qun Shen, NSLS-II Deputy for Science: and presentations from Ron Pindak, Stuart Wilkins, and Eric Dooryhee, NSLS-II Program Managers.

This year we have the special privilege of hearing from Bruce Garrett, Director Chemical Sciences, Geosciences, and Biosciences Division, about activities at the U.S. Department of Energy, as well as updates on activities at BNL from Doon Gibbs, at the NSLS-II from John Hill, and at the CFN from Chuck Black.

Also, this year we will be hosting nine scientific workshops, covering a broad range of topics. The NSLS-II and CFN Users’ Executive Committees and the Organizing Committee acknowledge the outstanding work of our workshop organizers: Daniel Allan, Nozomi Ando, Andi Barbour, Fernando Camino, Stuart Campbell, Thomas Caswell, Yu-chen Karen Chen-Wiegart, Yong Chu, Dean DeLongchamp, Mohamed Elbakshwan, Dan Fischer, James S. Fraser, Masa Fukuto, Oleg Gang, Eliot Gann, Simerjeet K. Gill, Wen Hu, Xiaojing Huang, Jeffrey Kysar, Claudio Mazzoli, Lisa Miller, Aleida Perez, George N. Phillips, Jr., Jurek Sadowski, Martin Schoonen, Robert Sweet, Juergen Thieme, Ruud Tromp, Elio Vescovo, Michael Wall, Stuart Wilkins, Garth Williams.

Finally, both UECs thank the amazing folks in the NSLS-II and CFN User Administration Offices and the BNL staff, all of whom do the hard work every year to provide us with a great Users’ Meeting.

We hope that you will enjoy all of the scientific and social events of the 2017 meeting!

Organizing Committee Members

Jeff Fitts, Meeting and Program Co-Chair, Princeton University
Don DiMarzio, Meeting and Program Co-Chair and Poster Chair, Northrop Grumman Corporation
Stanislaus Wong, Poster Chair, Stony Brook University
Kevin Yager, Workshop Chair, Brookhaven National Laboratory
Gretchen Cisco, NSLS-II User Administrator, Meeting Coordinator and Sponsor Chair, Brookhaven National Laboratory
Nancye Wright, Meeting Coordinator and Vendor Chair, Brookhaven National Laboratory
Grace Webster, CFN User Administrator, Brookhaven National Laboratory
Welcome
2017 Julian David Baumert Ph.D. Thesis Award
NSLS-II UEC Community Service Award
Student Scholarship Recipients
Main Meeting Agenda
Workshop 1
Multi-dimensional and Multi-modal X-ray Imaging and Analysis
Workshop 2
Spectro-microscopy at the Nanoscale: Exploring Chemical, Electronic and Magnetic Properties of Novel Materials
Workshop 3
Synchrotron Techniques in Support of DOE’s Subsurface R&D Effort
Workshop 4
Measurement and Interpretation of Diffuse Scattering in X-Ray Diffraction for Macromolecular Crystallography
Workshop 5
Bringing Big Science into the Classroom
Workshop 6
Polarized Resonant Soft X-ray Scattering at the NSLS-II
Workshop 7
Prospects in Imaging Materials and their Dynamics by Coherent X-ray Scattering
Workshop 8
Data Acquisition Cookbook: A Tutorial on NSLS-II’s Python DAQ Software
Workshop 9
Nano-mechanics: From Material Fabrication to In-Operando Characterization
BNL Site Map
Exhibitor and Sponsor Information
Location of Equipment and Instrumentation Exhibitors in Berkner Hall
Exhibitors at Workshops located at Chemistry Department, Bldg. 555
Exhibitors at Workshops located at CFN Department, Bldg. 735
Sponsors
Exhibitor Advertisements and Presentations
List of Equipment and Instrumentation Exhibitors
Accommodations
Offsite Transportation
Onsite Transportation
Nominees for the 2017-19 Users’ Executive Committee
This year’s Julian Baumert Thesis Award recipient is Kelli Hvorecny of Dartmouth College, who completed the requirements for her Ph.D. in March and will receive her degree in June. Hvorecny was chosen based on her work into the molecular mechanism and virulence of a protein secreted by the bacterium \textit{Pseudomonas aeruginosa} during its infection of airways, which she studied in part at beamline X6A of Brookhaven National Laboratory’s former National Synchrotron Light Source, a U.S. Department of Energy Office of Science User Facility, which has since been succeeded by the National Synchrotron Light Source II (NSLS-II). \textit{Pseudomonas aeruginosa} is widely present in the environment and resulting infections are most likely to strike hospital patients or those with weakened immune systems.

The Baumert award is given to a researcher who has recently conducted a thesis project that included measurements at NSLS or NSLS-II. It was established in memory of Julian David Baumert, a young Brookhaven physicist who was working on x-ray studies of soft-matter interfaces at NSLS before he died in June 2006.

Hvorecny’s adviser, Dean R. Madden, a professor in Dartmouth’s Department of Biochemistry & Cell Biology, calls her “a rising star, [who is] on track to become a leader in academic research and teaching.”

Hvorecny began her research just after the Madden group had identified one of the bacterium’s virulence factors (molecules that add to the overall infection potential of bacteria and viruses), known as CFTR inhibitory factor (Cif). It is named after a cell-membrane ion channel, the cystic fibrosis transmembrane conductance regulator (CFTR), that is defective in patients with cystic fibrosis (CF), a genetic condition that severely impairs the function of the lungs and digestive system. In particular, CFTR regulates the salt and water balance required for effective mucociliary clearance—the process by which inhaled bacteria are trapped in mucus, and then transported out of the airway by tiny hairs called cilia.

The group had found that Cif causes CFTR to undergo degradation after endocytosis, in which surface molecules, such as proteins, are internalized in vesicles that “pinch off” from the membrane. They reasoned that this degradation should enable Cif to interfere with mucociliary clearance, providing the bacterium with a way to infect people without CF. But, when Hvorecny joined the group, there were no data that directly tested this assumption. Additionally, and equally problematically, the group knew of no biological substrates that Cif would interact with to cause its effects.

With all of this in mind, Hvorecny first determined the crystal structures of some Cif mutants with various xenobiotic (foreign to the body) substrates, helping to uncover how it operates as an enzyme. This work was done at the NSLS and, through the NSLS transition program, at the Stanford Synchrotron Radiation Laboratory, another DOE Office of Science User Facility. Then, working from those structural insights, she identified a series of substrates among human fatty acids, including one that, quite surprisingly, modulates and helps to resolve inflammatory responses.

This work revealed a new pathway for the group’s research efforts and yielded a multi-university collaboration, which Hvorecny spearheaded. This partnership confirmed the inflammatory effect of Cif in cellular models and in airway samples from CF patients.

At the same time, Hvorecny was developing a new model for mucociliary transport in reconstituted epithelial cells, which make up the tissue that lines most cavities and surfaces of the body, such as the...
walls of blood vessels and organs. Also, by starting with a model of pneumonia in mice, she confirmed that Cif is a potent and rapid inhibitor of the body’s bacterial removal process.

Finally, she determined structures of Cif in complex with inhibitors that were found via a screening process and then coordinated a structure-based drug-design collaboration that found inhibitors with improved selectivity. The initial structure, from which the drug design was based, was the result of data taken at NSLS beamline X6A. 

“Like the best science, Kelli’s work brought clarity and understanding and, in doing so, uncovered brand-new areas of investigation,” said Madden. “She is a truly versatile scientist, but she is also a structural biologist’s structural biologist—always seeking better conditions, sweating the details of analysis, and training new students.”

The Baumert award will be presented during the 2017 NSLS-II and CFN Users’ Meeting. Kelli Hvorecny will receive a $600 honorarium and travel arrangements to Brookhaven National Laboratory.

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**UEC Community Service Award Recipient**

**Steve Bennett**

One of the great strengths of NSLS-II is the quality and creativity of the many staff members who provide technical and construction support. Truly it would be impossible to make science happen without all these terrific people. One person who really stands out among that crowd is Steve Bennett. As the technical support group leader, he directs a wonderful group of technicians. But what really sets Steve apart is his eager willingness to hear people’s problems and find quick solutions.

Just the other day at our beamline, we needed, of all things, a NEMA 5-20 power cable. Without it, we were stuck. Steve was riding by on his tricycle. We flagged him down and showed him the problem. 20 minutes later he came riding back with a spare cable for us to borrow.

I know the example I chose for this nomination is a very small thing, but it’s the kind of thing Steve does reflexively, always with a smile, and with unflagging good nature. He did that sort of thing for years back at NSLS and he continues to do so every day for people all around the ring. That he is a skilled technician ... well ... that’s his job description. That he always finds time to help people, that’s why he deserves this award. Another user added that “Steve is always cheerful and helpful. Even for things that aren’t directly under his supervision, he still makes every effort to get the info or provide a contact to get the job done.”

Steve Bennett started at Brookhaven National Laboratory in 1997 with the Superconducting Power Transmission Project. Steve moved to the AGS in 1980, the NSLS in 1983, and now NSLS-II. On behalf of the NSLS-II user community, we are pleased to recognize Steve with this award.
Two-Dimensional Models for Zeolites

*Nusnin Akter* a, JianQiang Zhong b, Mengen Wang a, John Kestell b, Dario Stacchiola b, Deyu Lu b, Taejin Kim a,c, J. Anibal Boscoboinik*b

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A model catalyst, from the surface science perspective, is a simpler version of a practical complex catalyst, with a well-defined structure of identifiable and countable sites, on a surface. The model is inspired by a real catalyst which helps to understand a catalytic phenomenon in more depth, in particular in regards to mechanistic aspects. Ultra-thin two-dimensional hexagonal (2dH) nanoporous (alumino)silicates have been synthesized on the Ru(0001) surface to mimic zeolites, which are the most used catalysts in the industry by volume. This 2dH model will help to understand the complex zeolite structure where the catalytically active sites are enclosed within the pores, which limits the fundamental understanding of the nature of active sites, reaction intermediate species, and molecular/electronic structure-performance relationships during experiment.

In this study, we explore the behavior of the 2D-model zeolite under elevated pressures. We observe that this model zeolite acts as atomic and molecular sieve which can trap Argon atoms within the nanopores and restricts the passage of CO molecules, preventing it adsorption on the Ru(0001) surface. Infrared Reflection Absorption Spectroscopy (IRRAS) at the CFN and Ambient Pressure X-ray Photoelectron Spectroscopy (AP-XPS) at the CSX-2 beamline of the NSLS-II were used for this study.

ACKNOWLEDGMENT: Research carried out in part at the CSX-2 beamline of the National Synchrotron Light Source II, Chemistry Department and Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-SC0012704. We gratefully acknowledge the financial support for this study from BNL LDRD 15-010, SBU/BNL SEED grant and the Department of Materials Science & Engineering at Stony Brook University through start-up research funding.
First Principles Study of Lithium Ion Batteries: Spinel Cathode Material

Haoyue Guo\textsuperscript{1} and Ping Liu\textsuperscript{2}

\textsuperscript{1}Department of Chemistry, Stony Brook University
\textsuperscript{2}Chemistry Department, Brookhaven National Laboratory

We report an extensive study on fundamental properties which determine the functional electrochemistry of ZnFe\textsubscript{2}O\textsubscript{4} spinel. For the first time, the reduction mechanism is followed through a combination of in-situ x-ray diffraction data, synchrotron based powder diffraction, ex-situ extended x-ray absorption fine structure (EXAFS) allowing complete visualization of reduction products irrespective of their crystallinity. The first 0.5 electron equivalents (ee) do not significantly change the starting crystal structure. Subsequent lithiation results in migration of Zn\textsuperscript{2+} ions from 8a tetrahedral sites into vacant 16c sites. Density Functional Theory shows that Li\textsuperscript{+} ions insert into 16c site initially and then 8a site with further lithiation. Fe metal is formed over the next 8 electron equivalents of reduction with no evidence of concurrent Zn\textsuperscript{2+} reduction to Zn metal. Despite the expected formation of LiZn alloy from the electron count, we find no evidence for this phase under the tested conditions. Additionally, upon oxidation to 3V, we observe an FeO phase with no evidence of Fe\textsubscript{2}O\textsubscript{3}. Electrochemistry data show higher electron equivalent transfer than can be accounted for solely based on ZnFe\textsubscript{2}O\textsubscript{4} reduction indicating excess capacity ascribed to carbon reduction or surface electrolyte interphase (SEI) formation.
**Ambient Pressure Activation of CO₂ on Titania Model Surfaces**

Rebecca Hamlyn¹, David C. Grinter⁶, Fang Xu⁵, Si Luo¹, Robert Palomino²,³, Iradwikanari Waluyo⁵, Dario J. Stacchiola⁴, Sanjaya D. Senanayake², José A. Rodriguez², Michael White¹,²

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² Chemistry Department, ³ National Synchrotron Light Source II, and ⁴ Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973
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CO₂ is utilized as a source for industrial methanol production (typically with CO and H₂ over Cu/ZnO/Al₂O₃) and is thus an attractive fuel synthesis feedstock, that allows for the mitigation of detrimental greenhouse effects. However, this catalytic conversion process over heterogeneous catalysts faces several challenges, including the chemical activation of CO₂, reaction stability and the knowledge of the active surface pathways remains poorly understood.

Recent catalytic studies have highlighted the importance of the metal and oxide interface as an essential component of catalyst for many reactions, and in the case of methanol synthesis, addition of reducible metal oxide nanoparticles to a metallic support have yielded orders of magnitude increases in activity [1-3]. The true nature of such systems remains unexplored.

We have started to study this reaction by a systematic study of the oxide support with CO₂. As titania is an economical, easily reduced and commonly utilized support, investigations into the activation of CO₂ were extended to a well-defined TiO₂(110) surface. Previous studies of CO₂ adsorption on titania model catalysts have been restricted to ultra high vacuum conditions [4], reflective of an ideal model reaction condition and separated in pressure to the real world reaction environment [2]. We have been able to bridge such reaction conditions by using a combination of ambient pressure X-ray Photoelectron Spectroscopy (AP-XPS) at the National Synchrotron Light Source II (23-ID-2 beamline) and AP-Scanning Tunneling Microscopy (AP-STM). We have studied the interaction of CO₂ on TiO₂(110) in the ambient pressure regime using both techniques and correlated the activation of CO₂ over the last layer of atoms of the TiO₂ surface. Atomically resolved images (AP-STM) show the adsorption of CO₂ along the Ti₅c rows, and the development of a stable adsorbate superstructure composed of many molecules of activated CO₂ at pressure. High resolution X-ray spectroscopic data (C₁s, O₁s) reveal the precise chemical state of the CO₂, and also identified the progressive oxidation of the titania surface with increasing pressure (Ti³⁺/Ti⁴⁺), indicating a reaction. We further studied the evolution of the surface species via reaction of a subset of the adsorbate species, and this species was seen to be stable even after evacuation of the CO₂ gas, typical for strong surface bonding. This suggests different surface binding sites and the possible interaction of co-adsorbates to heal the reduced oxygen vacancies of the catalytic surface. Subsequent investigation of more complex systems has begun on this model surface, with new or commonly used materials in the CO₂ conversion process. This includes the highly active copper component and the alkali promoter cesium.

Temperature Effects on the Microstructure of Saturated Kaolinite Clay

Karam A. Jaradat
Ph.D. student, Sustainable Geotechnics Laboratory, Department of Civil Engineering, Stony Brook University

This poster will present the research activities performed at CFN and NSLS-II investigating the temperature effects on the microstructure of saturated kaolinite clay. The research conducted at the Center of Functional Nanomaterials, at Brookhaven National Laboratory, utilized the dual FIB/SEM equipment to quantify the effects of elevated/freezing temperatures on clay microstructure, particularly, the evolution of the pore size distribution with temperature. The stack of 2-D SEM images generated from different clay samples prepared at different temperatures were used to reconstruct 3-D tomographies using Avizo Fire. The pore size distribution curve developed for freezing temperature showed an increase in the pore sizes compared to the reference sample at room temperature, which is justified by the expansion of pore water upon forming ice crystals. On the other hand, the heated clay sample showed an increase in the sizes of small pores and a reduction in the sizes of the large pores. This is explained by the anisotropic expansion of the clay particles as observed in the results of the XPD beamline at NSLS-II. At NSLS-II, the evolution of clay particles orientation and the expansion of the clay particles was investigated in-situ at temperatures ranging from -20 ºC to 90 ºC. The results of these in-situ experiments suggest that the thermal expansion coefficients of the clay particles in a direction parallel to the prism layers is higher than that in the direction parallel to the basal layers. Moreover, the thermally-induced particles re-orientation depends on the relative orientation of the particles and the thermally-induced pore water flow.
Lignocellulose is the most abundant raw material for biofuels and the most important bio-renewable resource for building materials, paper and textiles. A detailed understanding of the structure at nano- and meso-scale could accelerate the development of an efficient biofuel conversion method. The plant cell wall is a heterogeneous mixture of various complex biopolymers including cellulose, hemicellulose and pectin. The structure and assembly of these constituents in the plant cell wall is still not well understood. It is difficult to resolve the different elements through conventional hard X-ray scattering as they have similar electron density and hence, do not generate sufficient scattering contrast. The chemical specificity of resonant soft X-ray scattering (RSoXS) allows contrast to be generated based on differences in the chemistry of the different polysaccharides. By varying incident X-ray energies, we have achieved increased scattering contrast between cellulose and other polysaccharides from onions, such that features of the network structure of the cell wall are resolved. Thus, RSoXS reveals the packing distance of cellulose microfibrils embedded in the polysaccharide network. We have also performed grazing-incidence wide-angle X-ray scattering on different onion scales that reveals the orientation of cellulose fibers in the different scales.
Decorated, Crumpled Graphene Oxide Assemblies for MRI Contrast and Drug Delivery Agents

Shruti Sharma
Department of Materials Science and Chemical Engineering, Stony Brook University

Carbon nanomaterials (CNMs) are emerging as materials of interest in biological applications such as, drug delivery, and tissue imaging, and particularly with respect to their toxicity in cancer tissues. Graphene oxide based CNMs (GO-CNMs) possess notable geometrical variants, such as flat sheets, tubes, scrolls and spheres, and form stable and easily-processed aqueous solutions. Further, the presence of oxygen containing functional groups in GO-CNMs provide potential locations for attachment of drugs, disease targeting functional groups as well as decoration with metal nanoparticles, making them viable theranostics platforms. We synthesized mesoscale crumpled graphene oxide roses (GO roses) by using colloidal graphene oxide (GO) variants as precursors for a hybrid emulsification/rapid evaporation approach. This process produced rose-like, spherical, reduced mesostructures of colloidal graphene oxide, with corrugated surfaces. This synthesis route provides control over particle size, morphology and chemical properties of the synthesized GO roses. We investigated the morphology and chemical structure of these produced GO roses was using electron microscopy (SEM, TEM and FIB-assisted SEM) and spectroscopy techniques (FTIR, Raman and XPS) at the CFN. We are currently studying these synthesized mesostructures as potential theranostics platforms for cancer remediation as MRI contrast and drug delivery agents.
Fabrication and Characterization of an Amorphous Selenium Multi-Well Avalanche Photon Counting Detector for Breast Imaging

Jann Stavro\textsuperscript{a}, Amir H. Goldan\textsuperscript{a}, Ming Lu\textsuperscript{b}, Wei Zhao\textsuperscript{a}\textsuperscript{*}

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Jann.Stavro@stonybrook.edu (corresponding); Wei.Zhao@stonybrook.edu (*supervisor)

Photon counting detectors (PCDs) capable of energy discrimination have the potential to significantly improve medical x-ray imaging, however they are still hindered by several performance limitations and high production cost. Currently PCDs use crystalline semiconductors such as Cadmium Telluride and Silicon with fast carrier mobility and high charge conversion gain, however these materials suffer from low fabrication yields and structural defects. By using amorphous Selenium (a-Se) the cost of PCDs can be substantially reduced and enable large area deposition, while taking advantage of the inherent spatial resolution of a-Se. Typically amorphous materials are ruled out as viable candidates for temporally demanding detection tasks due to their slow carrier mobility. To circumvent this problem and the low charge conversion gain of a-Se we propose a novel detector structure called field-Shaping multi-Well Avalanche Detector (SWAD). SWAD divides the a-Se layer into two separate regions: (i) a thick (bulk) interaction region providing high detection efficiency and (ii) a thin (well) detection region. A set of grid electrodes within the well walls are biased to create field shaping in the a-Se, guiding the carriers from the bulk into the well. The focused electric field inside the well is an order of magnitude higher than that of the bulk, allowing avalanche multiplication to amplify the charge gain. Additionally the grid electrodes inside the well create a strong near field effect, enabling fast unipolar time differential (UTD) charge sensing. We have successfully fabricated the first practical multi-well structure, optimized for a direct conversion a-Se detector with avalanche gain. Our encouraging initial time of flight results successfully demonstrated UTD charge sensing, reinforcing the potential for SWAD to be a successful PCD design. SWAD would be the first large area 2D PCD system capable of stable avalanche gain and fast timing.

Acknowledgements:

We acknowledge financial support from the National Institutes of Health (R21 EB019526 and R01 EB002655). Research on SWAD fabrication was carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-SC0012704.
Mesoporous cobalt-ceria catalysts are being investigated for their activity in the water-gas shift reaction. Catalysts were prepared via in-situ doping, a process which utilizes a recently developed sol-gel synthesis method for mesoporous materials, yielding monomodal 3-4 nm ceria crystallites with interparticle pores which could be tuned with calcination temperature. In-situ X-ray diffraction XRD experiments on the mesoporous Co/CeO2 system demonstrated changes in ceria lattice behavior indicative of a degree of doping, however no crystalline cobalt phases were observed with Co loadings up to 10%, prompting a closer investigation into the state of the cobalt component. Soft X-ray absorption spectroscopy was performed at NSLS-II beamline 23-ID-2 (CSX-2), which yielded identification of a Co2+ state in the mesoporous Co/CeO2 catalysts. An in-situ Co K-Edge XANES study was performed at NSLS-II beamline 8-ID (ISS), with results indicating partial reduction of Co2+ to metallic cobalt under reaction conditions. Surface reactivity was further probed using in-situ infrared (DRIFTS) and ambient pressure X-ray photoelectron spectroscopy under water-gas shift reaction conditions. This study presents a comprehensive analysis of the structural and chemical states of mesoporous Co/CeO2 catalysts during the water-gas shift reaction.
First Principles Study of the Interface Structure and Charge Compensation at the Aluminosilicate / Ru(0001) Heterojunction

Mengen Wang a,b, Jianqiang Zhong a, J. Anibal Boscoboinik * a, Deyu Lu * a

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b Department of Materials Science and Chemical Engineering, Stony Brook University

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Two-dimensional (2D) ultrathin aluminosilicate films, consisting of aluminosilicate bilayer films weakly bound to the Ru(0001) surface, have been synthesized as a model system for heterogeneous catalysis studies for zeolite chemistry. Understanding the interface structure and charge redistribution at the aluminosilicate/Ru(0001) heterojunction is a fundamental step to unravel the structure-function relationship that is essential to the design of new catalysts. In-situ X-ray photoelectron spectroscopy (XPS) measurements found that the O 1s core-level binding energy in aluminosilicate films is lower than that in silica films at low surface O coverage. We carried out van der Waals density functional theory (vdW-DFT) calculations of the aluminosilicate/Ru(0001) heterojunction. Our calculations revealed that the lower O 1s core-level binding energy in aluminosilicate films is caused by the charge compensation at the interface that modifies interface dipole moments. The charge rearrangement at the interface results from the electron transfer from the substrate to the film and the atomic orbital hybridization between O $p_z$ and Ru $d_{xz}$ states. The chemisorbed O atoms on Ru(0001) can block the charge compensation at the interface. During the oxidation of the Ru(0001) surface, changes in the surface and interface dipole moments move the O 1s core-level closer to the Fermi level, which is consistent with experimental results.

This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704. M.W. and J.Z. are supported by BNL LDRD Project No. 15-010.
Diamond has been proven to be a perfect material for X-ray monitoring due to its unique properties, such as low absorption, high thermal conductivity and large bandgap. Diamond detectors are typically made from 50~500 µm thick intrinsic single crystal diamonds with 30 nm platinum deposited on both sides, thus forming a double sided Schottky barrier diode. In most cases, the diamond detector works well in transmission mode, which means the detector is installed upstream of the sample and gives the real-time incident flux. Operation in transmission is a unique feature of diamond detectors which is not possible with traditional Si-based devices. But in the soft X-ray regime (500~2000 eV), a 50 µm diamond fully absorbs the beam. Therefore, thinner diamonds (~5 µm) are needed for soft X-ray monitoring while working in transmission mode. Laser slicing and polishing can thin diamonds to around 30 µm. For further thinning, deep reactive ion etching work is utilized. Deep etching on diamonds while keeping a smooth and flat surface is challenging since the bulk diamond contains some residual internal strain, and defects in diamonds can emerge as roughness or pits. We have successfully made several diamond membrane (5-10 µm) detectors and demonstrated them to work properly at the SMI beamline at NSLS-II. Together with lithographically defined Pt electrodes, the diamond membrane detectors provided soft x-ray flux and position information. Furthermore, the thin diamond membrane lowers the nitrogen impurity requirement for diamonds used as diodes. In this poster, the fabrication process and testing results of the membranes are included.
As radiation therapy develops, such as gamma ray therapy and particle therapy, new types of radiation tolerant detectors are required to enable accurate measurement of beam flux, position and timing which will ensure the intended dose is delivered. Diamond, widely known as its high radiation hardness, high thermal conductivity, high speed and low intrinsic carrier density, has great potential in radiation detection of therapeutic beams. To test diamond lifetime in proton radiation and performance after radiated, we have irradiated several diamond detectors with an 800MeV proton beam at the LANSCE facility at the Los Alamos National Laboratory. The total delivered dose was equivalent to ~100 years of clinical exposure. The proton beam was controlled to be intermittently injected while the real-time ion beam induced current (IBIC) was monitored during exposure. We observed an exponential decay in the response of all detectors with a $1/e$ decay time equivalent to 30 years of clinical dose. Also, we have utilized X-ray beam induced current (XBIC, including both monochromatic beam and white beam) for detector performance testing before and after proton radiation, measuring response uniformity and flux calibration. The decreasing responses observed in all detectors are attributed to carrier traps induced from proton radiation damage. The reduced response varied smoothly across the active area of the detector arising from being exposed using the side of the Gaussian distribution of proton beam. Some damage variations were confirmed by simulation to be the result of elastic scattering. Further investigations are underway to determine the nature of the radiation damage.
# Agenda

## Sunday, May 14, 2017

<table>
<thead>
<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>4:00 p.m.</td>
<td>7:00 p.m.</td>
<td>Optional Vendor and Poster Set Up</td>
<td>Berkner Hall Lobby and Cafeteria</td>
</tr>
<tr>
<td>4:00 p.m.</td>
<td>7:00 p.m.</td>
<td>Early Registration - Registration Office Opens</td>
<td>Berkner Hall Lobby and Room D</td>
</tr>
</tbody>
</table>

## Monday, May 15, 2017

<table>
<thead>
<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:00 a.m.</td>
<td>5:00 p.m.</td>
<td>Registration Office Opens – all attendees must check in before attending any event</td>
<td>Berkner Hall Lobby and Room D</td>
</tr>
<tr>
<td>7:30 a.m.</td>
<td>4:00 p.m.</td>
<td>Vendor Exhibit and Poster Set Up</td>
<td>Berkner Hall Lobby and Cafeteria</td>
</tr>
<tr>
<td>8:50 a.m.</td>
<td>5:20 p.m.</td>
<td><strong>Workshop 1:</strong> Multi-dimensional and Multi-modal X-ray Imaging and Analysis</td>
<td>Berkner Hall, Bldg. 488, Conf. Room B</td>
</tr>
<tr>
<td>8:30 a.m.</td>
<td>5:30 p.m.</td>
<td><strong>Workshop 2:</strong> Spectro-microscopy at the Nanoscale: Exploring Chemical, Electronic and Magnetic Properties of Novel Materials</td>
<td>CFN, Bldg. 735, Large Conf. Room</td>
</tr>
<tr>
<td>8:50 a.m.</td>
<td>5:30 p.m.</td>
<td><strong>Workshop 3:</strong> Synchrotron Techniques in Support of DOE’s Subsurface R&amp;D Effort</td>
<td>Computational Science, Bldg. 725, Seminar Room</td>
</tr>
<tr>
<td>8:30 a.m.</td>
<td>5:30 p.m.</td>
<td><strong>Workshop 4:</strong> Measurement and Interpretation of Diffuse Scattering in X-Ray Diffraction for Macromolecular Crystallography</td>
<td>Chemistry, Bldg. 555, Hamilton Seminar Room</td>
</tr>
<tr>
<td>12:30 p.m.</td>
<td>1:30 p.m.</td>
<td>Lunch Break (included - luncheon ticket required)</td>
<td>Workshop Locations</td>
</tr>
<tr>
<td>4:30 p.m.</td>
<td>5:30 p.m.</td>
<td>NSLS-II Tours - sign up at registration desk</td>
<td>Berkner Hall Conf. Room D</td>
</tr>
<tr>
<td>5:30 p.m.</td>
<td></td>
<td>All Workshops Conclude</td>
<td>Workshop Locations</td>
</tr>
<tr>
<td>Time</td>
<td>Event</td>
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<tr>
<td>5:30 p.m.</td>
<td>Registration Office Closes</td>
<td>Berkner Hall Conf. Rm. D</td>
<td></td>
</tr>
<tr>
<td>5:30 p.m.</td>
<td>7:30 p.m.</td>
<td>Discovery Park and BNL Quality of Life/Infrastructure</td>
<td>Berkner Hall Lobby</td>
</tr>
<tr>
<td>5:30 p.m.</td>
<td>7:30 p.m.</td>
<td>Welcome Reception, Vendor Exhibit and Poster Session</td>
<td>Berkner Hall Lobby and Cafeteria</td>
</tr>
</tbody>
</table>

**NSLS-II Tours**

Come see the new exciting happenings at NSLS-II!

Tours will be held on Monday and Tuesday
Starting at 4:30 pm - 5:30 pm

Sign up at the registration desk in Conf. Rm. D, Berkner Hall.

**Welcome Reception, Exhibitor and Poster Session**

**Monday, May 15, 2017 - 5:30 pm - 7:30 pm**

Come join us for an opportunity to view the exhibits and network with over 50 NSLS-II and CFN vendors. Also, more than 50 posters, submitted by scientists, researchers, post docs and students exhibiting their research at the NSLS, NSLS-II and CFN, will be on display. The Poster Session will open Monday, May 15, at 5:30 p.m. and close Wednesday, May 17, at 12:00 p.m. It will be located in close proximity to the vendor instrumentation/equipment exhibit and refreshments.

Heavy hors-d’oeuvres and refreshments will be served.

Registered attendees (general and student) receive one ticket to the Welcome Reception, compliments of our sponsors and exhibitors. Additional tickets (guests and free plenary registration) may be purchased for $20.
# NSLS-II & CFN Users’ Meeting

**May 15-17, 2017**

## Agenda

**Tuesday, May 16, 2017**

<table>
<thead>
<tr>
<th>Starts</th>
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<th>Event</th>
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<tbody>
<tr>
<td>7:30 a.m.</td>
<td>5:00 p.m.</td>
<td>Registration Office Opens ~ all attendees must check in before attending any event</td>
<td>Berkner Hall Lobby and Room D</td>
</tr>
<tr>
<td>8:00 a.m.</td>
<td>5:00 p.m.</td>
<td>Vendor Exhibit and Poster Session</td>
<td>Berkner Hall Lobby and Cafeteria</td>
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</tbody>
</table>

### Early Morning Plenary Session

Open to all, free of charge (registration is required)
(8:30 a.m. to 10:55 a.m.)

Session Chair, Donald Weidner
Distinguished Professor, Stony Brook University
Chair, NSLS-II Users’ Executive Committee

<table>
<thead>
<tr>
<th>Starts</th>
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<tbody>
<tr>
<td>8:30 a.m.</td>
<td>8:35 a.m.</td>
<td>“Welcome”</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>8:35 a.m.</td>
<td>8:55 a.m.</td>
<td>“BNL Update”</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>8:55 a.m.</td>
<td>9:40 a.m.</td>
<td>“BES Update”, Bruce Garrett, Director, Chemical Sciences, Geosciences, &amp; Biosciences Division, U.S. Department of Energy, Office of Basic Energy Sciences</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>9:40 a.m.</td>
<td>10:25 a.m.</td>
<td>“Keynote Talk”, Teri W. Odom, Charles E. and Emma H. Morrison Professor; Associate Chair of the Department of Chemistry, Northwestern University</td>
<td>Berkner Hall Auditorium</td>
</tr>
</tbody>
</table>

### Morning Break - Continental Breakfast (included)

(10:25 a.m. to 10:55 a.m.)

<table>
<thead>
<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
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<tbody>
<tr>
<td>10:25 a.m.</td>
<td>1:30 p.m.</td>
<td>Discovery Park and BNL Quality of Life/Infrastructure</td>
<td>Berkner Hall Lobby</td>
</tr>
<tr>
<td>10:25 a.m.</td>
<td>12:15 p.m.</td>
<td>BNL Exhibitors Networking Session and Presentations (Open to all BNL)</td>
<td>Berkner Hall Lobby and Cafeteria</td>
</tr>
<tr>
<td>10:25 a.m.</td>
<td>10:35 a.m.</td>
<td>Photo: NSLS-II/CFN UEC Members, BNL and DOE Management</td>
<td>Berkner Hall</td>
</tr>
<tr>
<td>10:35 a.m.</td>
<td>10:45 a.m.</td>
<td>Photo: Users’ Meeting Planning Committee</td>
<td>Berkner Hall</td>
</tr>
</tbody>
</table>
# Late Morning Plenary Session
Open to all, free of charge (registration is required)
(10:55 a.m. to 12:15 p.m.)

Session Chair, Jeff Fitts, Research Scholar, Princeton University
Vice Chair, NSLS-II Users’ Executive Committee

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<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
<th>Location</th>
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<tbody>
<tr>
<td>10:55 a.m.</td>
<td>11:25 a.m.</td>
<td>“NSLS-II Update”, John Hill, Deputy ALD for Energy Sciences &amp; Photon Sciences and Director of NSLS-II, Brookhaven National Laboratory</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>11:25 a.m.</td>
<td>11:45 a.m.</td>
<td>“NSLS-II Strategic Plan Update”, Qun Shen, Deputy for Science, NSLS-II, Brookhaven National Laboratory</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>11:45 a.m.</td>
<td>12:05 p.m.</td>
<td>“Soft X-ray Scattering and Spectroscopy Research Program Update”, Stuart Wilkins, Program Manager, NSLS-II, Brookhaven National Laboratory</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>12:05 p.m.</td>
<td>12:15 p.m.</td>
<td>UEC Election Results</td>
<td>Berkner Hall Auditorium</td>
</tr>
</tbody>
</table>

# Lunch Break
(Luncheon Ticket Required)
(12:15 p.m. to 1:30 p.m.)

<table>
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<tr>
<th>Starts</th>
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<th>Location</th>
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<tbody>
<tr>
<td>12:15 p.m.</td>
<td>1:30 p.m.</td>
<td>Joint UEC lunch with, Bruce Garrett, Director Chemical Sciences, Geosciences, &amp; Biosciences Division, U.S. Department of Energy, Office of Basic Energy Sciences</td>
<td>Berkner Hall Conf. Rm. A</td>
</tr>
</tbody>
</table>

# Early Afternoon Plenary Session
Open to all, free of charge (registration is required)
(1:30 p.m. to 2:45 p.m.)

Session Chair, Stanislaus Wong
Professor, Department of Chemistry, Stony Brook University
Chair, CFN Users Executive Committee

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<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>1:30 p.m.</td>
<td>4:00 p.m.</td>
<td>BNL Exhibitors Networking Session and Presentations (Open to BNL)</td>
<td>Berkner Hall Lobby and Cafeteria</td>
</tr>
<tr>
<td>1:30 pm</td>
<td>2:00 pm</td>
<td>“CFN Update”, Charles Black, Director, Center for Functional Nanomaterials, Brookhaven National Laboratory</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>2:00 pm</td>
<td>2:40 pm</td>
<td>Plenary Talk 1: “Synchrotron Based in situ Characterization during Atomic Layer Deposition”, Christophe Detavernier, Professor, Ghent University</td>
<td>Berkner Hall Auditorium</td>
</tr>
</tbody>
</table>

# Afternoon Break (included)
(2:45 p.m. to 3:05 p.m.)
Late Afternoon Plenary Session
Open to all, free of charge (registration is required)
(3:05 p.m. to 5:00 p.m.)
Session Chair, Don DiMarzio, Senior Scientist & Engineering Fellow, Northrop Grumman Corp.
Vice Chair, CFN Users’ Executive Committee

<table>
<thead>
<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
<th>Location</th>
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<tbody>
<tr>
<td>3:05 p.m.</td>
<td>3:50 p.m.</td>
<td>Plenary Talk 2: “XPCS: Past, Present and Future”, Mark Sutton, Professor, McGill University</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>3:50 p.m.</td>
<td>4:10 p.m.</td>
<td>“Complex Scattering Research Program Update”, Ron Pindak, Program Manager, NSLS-II, Brookhaven National Laboratory</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>4:10 p.m.</td>
<td>4:30 p.m.</td>
<td>“Diffraction and In-Situ Scattering Research Program Update”, Eric Dooryhee, Program Manager, NSLS-II, Brookhaven National Laboratory</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>4:30 p.m.</td>
<td>4:45 p.m.</td>
<td>Poster Winners and Community Service Award</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>4:30 p.m.</td>
<td>5:30 p.m.</td>
<td>NSLS-II Tours - sign up at registration desk</td>
<td>Berkner Hall Conf. Rm. D</td>
</tr>
<tr>
<td>4:45 p.m.</td>
<td>5:00 p.m.</td>
<td>Julian David Baumert Ph.D. Thesis Award</td>
<td>Berkner Hall Auditorium</td>
</tr>
<tr>
<td>5:00 p.m.</td>
<td>5:30 p.m.</td>
<td>NSLS-II UEC Meeting</td>
<td>Berkner Hall Conf. Rm. B</td>
</tr>
<tr>
<td>5:00 p.m.</td>
<td>5:30 p.m.</td>
<td>CFN UEC Meeting</td>
<td>Berkner Hall Conf. Rm. A</td>
</tr>
<tr>
<td>5:30 p.m.</td>
<td></td>
<td>Board bus to Giorgio’s in Baiting Hollow</td>
<td>Outside Berkner Hall</td>
</tr>
<tr>
<td>5:40 p.m.</td>
<td></td>
<td>Pickup at bldg. 740 (tour attendees)</td>
<td>Outside Bldg. 740</td>
</tr>
<tr>
<td>5:45 p.m.</td>
<td></td>
<td>Bus leaves BNL to Giorgio’s in Baiting Hollow</td>
<td></td>
</tr>
<tr>
<td>6:15 p.m.</td>
<td>9:45 p.m.</td>
<td>Users’ Meeting Annual Banquet (Giorgio’s)</td>
<td>Baiting Hollow, NY</td>
</tr>
<tr>
<td>9:45 p.m.</td>
<td></td>
<td>Bus departs Giorgios to BNL</td>
<td></td>
</tr>
</tbody>
</table>

**Don’t Miss This Year’s Annual Users’ Meeting Banquet**
**Tuesday, May 16, 2017**
**6:15 pm - 9:45 pm**

This year’s banquet will be held off-site at Giorgios in Baiting Hollow, NY. Lots of food will be on the menu, so bring your appetite!

The annual banquet is a great opportunity to relax and take pleasure in the company of your colleagues and associates while enjoying great food.

There will be a Jazz Performance by Kickback Trio and an after dinner presentation by Professor Robert Crease, titled “How Synchrotron Light Conquered Brookhaven”.

Professor Crease is with the Department of Philosophy, Stony Brook University. He is also a Columnist for Physics World and Co-Editor-in-Chief for Physics in Perspective.

Roundtrip transportation (first come, first serve) to the banquet venue will be provided.

The cost is $50.00 (general); $25.00 (student).

If you have not registered and would like to attend the banquet, please see someone in the registration office. We really hope you can join us for this special night out!
## Agenda

**Wednesday, May 17, 2017**

<table>
<thead>
<tr>
<th>Starts</th>
<th>Ends</th>
<th>Event</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>8:00 a.m.</td>
<td>1:30 p.m.</td>
<td>Registration Office Opens ~ all attendees must check in before attending any event</td>
<td>Berkner Hall Conf. Room D</td>
</tr>
<tr>
<td>9:00 a.m.</td>
<td>5:00 p.m.</td>
<td><strong>Workshop 5:</strong> Bringing Big Science into the Classroom</td>
<td>Computational Science, Bldg. 725, Seminar Room</td>
</tr>
<tr>
<td>8:30 a.m.</td>
<td>12:30 p.m.</td>
<td><strong>Workshop 6:</strong> Polarized Resonant Soft X-ray Scattering at the NSLS-II</td>
<td>Berkner Hall, Bldg. 488, Conference Room B</td>
</tr>
<tr>
<td>9:00 a.m.</td>
<td>5:00 p.m.</td>
<td><strong>Workshop 7:</strong> Prospects in Imaging Materials and their Dynamics by Coherent X-ray Scattering</td>
<td>Physics, Bldg. 510, Large Seminar Room</td>
</tr>
<tr>
<td>1:00 p.m.</td>
<td>5:00 p.m.</td>
<td><strong>Workshop 8:</strong> Data Acquisition Cookbook: A Tutorial on NSLS-II’s Python DAQ Software</td>
<td>Berkner Hall, Bldg. 488, Conference Room B</td>
</tr>
<tr>
<td>8:30 a.m.</td>
<td>5:00 p.m.</td>
<td><strong>Workshop 9:</strong> Nano-mechanics: From Material Fabrication to In-Operando Characterization</td>
<td>CFN, Bldg. 735, Large Conf. Rm.</td>
</tr>
<tr>
<td>12:00 p.m.</td>
<td></td>
<td>Exhibitor raffle prizes awarded</td>
<td>Berkner Hall Conf. Rm. D</td>
</tr>
<tr>
<td>12:30 p.m.</td>
<td>1:30 p.m.</td>
<td>Lunch Break - (included - Luncheon ticket required)</td>
<td>Workshop Locations</td>
</tr>
<tr>
<td>1:30 p.m.</td>
<td></td>
<td>Registration Office Closes</td>
<td>Berkner Hall Conf. Room D</td>
</tr>
<tr>
<td>5:00 p.m.</td>
<td></td>
<td>All Workshops conclude</td>
<td>Workshop Locations</td>
</tr>
</tbody>
</table>
Workshop 1  
Multi-dimensional and Multi-modal X-ray Imaging and Analysis  
May 15, 2017

Location: Berkner Hall, Bldg. 488, Conference Room B

Organizers: Yu-chen Karen Chen-Wiegart, Stony Brook U. and NSLS-II-BNL (ycchen@bnl.gov)  
Lisa Miller, NSLS-II-BNL (lmiller@bnl.gov)  
Juergen Thiem, NSLS-II-BNL (thieme@bnl.gov)  
Yong Chu, NSLS-II-BNL (ychu@bnl.gov)  
Thomas Caswell, NSLS-II-BNL (tcaswell@bnl.gov)  
Stuart Campbell, NSLS-II-BNL (scampbell@bnl.gov)

Description: Multi-dimensional and multi-modal imaging is a powerful research approach. Multi-dimensional imaging includes techniques such as tomography, spectroscopic microscopy, or in situ/operando imaging, enabling the characterization of samples in 3D spatially, with chemical sensitivity, and/or in a time-resolved fashion. Multi-modal imaging combines imaging techniques across different length-scales with different contrast mechanisms or with other interaction mechanisms, such as diffraction or scattering. This can provide unprecedented analysis of samples on multi-length scales or with enriched information.

This powerful research approach, however, faces challenges in particular on data analysis. For the complex nature of the multi-dimensional and multi-modal imaging, data collection, analysis, quantification and visualization tools need to be further developed in the scientific community and specifically at NSLS-II. Focusing on synchrotron x-ray imaging, this workshop aims to bring together the external experts on four specific themes and to facilitate in-depth discussions on these challenges with NSLS-II and the user community: 1) Grand challenges on multi-dimensional and multi-modal imaging and analysis, 2) Improvement on multi-dimensional and multi-modal data collection and pre-processing, 3) Multi-modal contrast & length scale registration and correlation, and 4) Quantification, visualization and modeling in multi-dimensional and multi-modal imaging.

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>8:35 a.m.</td>
<td>Continental Breakfast (included)</td>
</tr>
<tr>
<td>8:50 a.m.</td>
<td>“Introduction/Welcome to the Workshop”</td>
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<tr>
<td></td>
<td>Karen Chen-Wiegart, Stony Brook University and Brookhaven National Laboratory</td>
</tr>
<tr>
<td>9:00 a.m.</td>
<td>Theme I: Grand Challenges on Multi-dimensional and Multi-modal Imaging and Analysis</td>
</tr>
<tr>
<td>9:00 a.m.</td>
<td>“Grand Challenges of Multi-dimensional and Multi-modal Imaging and Analysis at NSLS-II”</td>
</tr>
<tr>
<td></td>
<td>Stuart Campbell, NSLS-II, Brookhaven National Laboratory</td>
</tr>
<tr>
<td>9:30 a.m.</td>
<td>“Multi-dimensional and Multi-modal Imaging and Analysis at the Diamond Light Source”</td>
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<td></td>
<td>Mark Basham, Diamond Light Source Ltd.</td>
</tr>
<tr>
<td>10:00 a.m.</td>
<td>“Discussions on Theme I”</td>
</tr>
<tr>
<td></td>
<td>Lisa Miller, Brookhaven National Laboratory</td>
</tr>
<tr>
<td>10:30 a.m.</td>
<td>Morning Break (included)</td>
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</table>

Theme II: Improvement on Multi-dimensional and Multi-modal Data Collection and Pre-processing
<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Speaker</th>
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</thead>
<tbody>
<tr>
<td>11:00 a.m.</td>
<td>“X-ray Fluorescence Computed Tomography: Novel Reconstruction Algorithms and Acquisition Strategies”</td>
<td>Patrick La Riviere, University of Chicago</td>
</tr>
<tr>
<td>11:30 a.m.</td>
<td>“Data Alignment in X-ray Nano-tomography”</td>
<td>Doga Gursoy, Argonne National Laboratory</td>
</tr>
<tr>
<td>12:00 p.m.</td>
<td>“Discussions on Theme II”</td>
<td>Yong Chu, NSLS-II, Brookhaven National Laboratory</td>
</tr>
<tr>
<td>12:30 p.m.</td>
<td>Lunch (included)</td>
<td></td>
</tr>
<tr>
<td>1:30 p.m.</td>
<td>“An Overview of Multi-dimensional, Multi-modal, Image Registration Methods and their Application with the Insight Toolkit (ITK) and Tomviz”</td>
<td>Matthew McCormick, Kitware, Inc.</td>
</tr>
<tr>
<td>2:00 p.m.</td>
<td>“Data Mining in Correlative Multi-modal X-ray Microscopy”</td>
<td>Yijin Liu, Stanford Synchrotron Radiation Lightsource</td>
</tr>
<tr>
<td>2:30 p.m.</td>
<td>“Discussions on Theme III”</td>
<td>Stuart Campbell, NSLS-II, Brookhaven National Laboratory</td>
</tr>
<tr>
<td>3:00 p.m.</td>
<td>Coffee break (included) and Group Photo</td>
<td></td>
</tr>
<tr>
<td>3:30 p.m.</td>
<td>“Easy Integrated Analysis and Visualization of Multi-modal and Multi-dimensional Image and Spectral Data with Dragonfly”</td>
<td>Mike Marsch, Object Research Systems, Inc.</td>
</tr>
<tr>
<td>4:00 p.m.</td>
<td>“High Throughput Reverse Image Search with pyCBIR: Quantification, Search, Retrieval and Ranking for Multi-modal Imaging”</td>
<td>Daniela Ushizima, Lawrence Berkeley National Laboratory</td>
</tr>
<tr>
<td>4:30 p.m.</td>
<td>“Discussions on Theme IV”</td>
<td>Thomas Caswell, NSLS-II, Brookhaven National Laboratory</td>
</tr>
<tr>
<td>5:00 p.m.</td>
<td>“Conclusion Remark and Summary from Discussions”</td>
<td>Karen Chen-Wiegart, Stony Brook University and Brookhaven National Laboratory</td>
</tr>
<tr>
<td>5:20 p.m.</td>
<td>Workshop Concludes</td>
<td></td>
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</table>

9:00 a.m. “Grand Challenges of Multi-dimensional and Multi-modal Imaging and Analysis at NSLS-II”
Stuart Campbell, NSLS-II, Brookhaven National Laboratory

The National Synchrotron Light Source II (NSLS-II) is the newest, highly optimized third-generation synchrotron facility in the world. In this talk, we will present an overview of the NSLS-II together with some of the challenges we are facing in order to perform multi-modal and multi-dimensional data collection and analysis. This will mainly focus on the IT and software aspects of the problem. It is intended to pose questions, such as, do we fully understand all aspects of what we need, what solutions already exist and where can we work together to find a solution.

9:30 a.m. “Multi-dimensional and Multi-modal Imaging and Analysis at the Diamond Light Source”
Mark Basham, Diamond Light Source Ltd.

Diamond Light Source has been collecting full field tomography data for over 9 years, and during this time the methodologies for dealing with the large quantities of data collected have changed dramatically. Initially much effort was spent optimising a sinogram based reconstruction methodology, where hdf5 and the NeXus format were employed to divide the whole reconstruction process into sinograms from the start, and then to process them using a batch processing cluster approach. Although this was effective, science drivers such
as the Paganin filter, and multi-modal data collections meant that this simple approach was too restrictive to be extended to these new methodologies. In the last 2 years, Diamond has started collecting greater numbers of time resolved tomography datasets, and multi-modal XRF, XRD and absorption chemical tomography datasets. In preparation for this over the last 3 years Diamond has tried to address these complex problems by creating a generic, extensible, scalable and standardized pipeline for processing all types of multi-dimensional and multi-modal data, Savu. As a pipeline, Savu tries to make use of as many existing libraries as possible by wrapping them as plugins in the framework, currently making use of the Astra toolbox, tomopy's gridrec, pyMCA, Pyfai, PtyPy, scikit image and many others. The framework itself deals with organizing the data and running all of the potentially single threaded or GPU optimised codes across cluster resources when available. Datasets can be processed independently or in combination, such as using absorption data to correct the reconstructions of XRF and XRD datasets, and processing steps can be chained together in any sensible way. Savu has been successfully used to process terabyte sized raw data files of time resolved tomography data, as well as chemical tomography datasets, and Ptycho-Tomographic data, and is in routine use on 5 beamlines at Diamond Light Source. In addition its open source nature and use of standard libraries such as python, HDF5 and MPI, has meant its successful installation on several cluster and stand-alone systems.

11:00 a.m.  "X-ray Fluorescence Computed Tomography: Novel Reconstruction Algorithms and Acquisition Strategies"
Patrick La Riviere, University of Chicago

X-ray fluorescence tomography allows for three-dimensional mapping of trace metals in intact samples. It presents numerous challenges for image reconstruction, including the need to correct for fluorescence self-absorption in the absence of needed attenuation maps. We will discuss efforts by us and others to address this problem, as well as alternative acquisition geometries that minimize the self-absorption problem. In addition, we will discuss efforts to perform lower-resolution XFCT using position- and energy-sensitive cameras coupled with collimating apertures that eliminate the need for full tomographic reconstruction and allow for direct region of interest imaging.

11:30 a.m.  "Data Alignment in X-ray Nano-tomography"
Doga Gursoy, Argonne National Laboratory

As x-ray tomography is pushed farther into the nanoscale, the limitations of rotation stages become more apparent leading to challenges in the processing of the acquired projection images. Here, I will present approaches for rapid post-acquisition alignment of these measurements to obtain high quality 3D images, and show its application in x-ray nano-tomography

1:30 p.m.  "An Overview of Multi-dimensional, Multi-modal, Image Registration Methods and their Application with the Insight Toolkit (ITK) and Tomviz"
Matthew McCormick, Kitware, Inc.

New scientific insights into materials are possible when information from images obtained with multiple modalities or at multiple scales are combined. Registration through automated or semi-automated software algorithms enables quantification and visualization of multi-dimensional and multi-modal image information.

In this talk, first we describe challenges in this analysis domain, including variations in voxel intensities, noise, and artifacts across modalities. Another challenge is divergence in structure features at different scales.

Next, we describe approaches to the multi-modal registration problem. These include mutual information-based image similarity metrics, registration of segmented structures, and registration of feature points.

Finally, we describe how these approaches can be applied with algorithms implemented in the open-source, Python-wrapped Insight Toolkit (ITK). We describe how they can be applied in Tomviz, an open source application for materials science and tomography based on the Visualization Toolkit (VTK), ParaView, ITK, and Python.
The studies of structurally complex and chemically heterogeneous systems usually require a suite of analytical tools that are capable of providing complementary information. X-ray microscopy offers several different imaging modalities that probe structural and chemical information through different contrast mechanisms at different length scales. As a result, X-ray microscopy has been recognized as a powerful tool for researches across different scientific disciplines.

In this presentation, the strength of correlative multi-modal X-ray microscopy will be highlighted through brief discussion of a few scientific case studies including the researches in geoscience [1] and petroleum industry [2]. The information extraction aspect of these researches will be emphasized. More recent developments in the data mining associated with the spectro-microscopy will also be discussed by presenting case studies in energy material research [3].

References
Shi et al., Nat. Geosci. 6, 971–975 (2013); Liu et al., in prep.

Dragonfly is a commercially available software platform for interactive inspection, analysis, and segmentation of image data. By design, the platform lets users integrate data from multiple sources where various datasets or image channels can be overlaid for visualization and analysis. This is true for datasets which may be fully overlapping, partially overlapping, or not overlapping at all, even in cases those data sets may be acquired in different coordinate systems and at different imaging resolutions. Because those datasets coexist in space in one framework, it becomes very easy to take advantage of all of the different signals for interpreting the materials being studied, and all of the composite channels can contribute to the image segmentation approach.

When Dragonfly was developed, a major design decision was made about how to balance performance-intensive compute and visualization subroutines with application logic. The former is developed in C++ with the help of system-level drivers, such as OpenGL and OpenCL, while the latter is developed in Python. By developing the application control in Python, Dragonfly has the advantage that maintenance and advancement of features can happen rapidly. Furthermore, an expansive library of image processing tools in Python is available for the development of advanced features by both the company’s developers and end-users working on plugins. Developers have multiple access points we call sockets, where custom code can be inserted and resulting modules behave as peers to factory-developed modules. One of the strongest advantages of the Python integration is a built-in console that lets developers prototype and test algorithms directly in the application in a style similar to usage patterns used by MATLAB developers.

In this talk, we will report on our progress for dealing with high-dimensional datasets. In collaboration with partners, we have adopted a general-purpose file format for handling large multi-dimensional datasets. We also now support data structures for n-dimensional data that are consistent with Numeric Python arrays, enabling disk-access for data that are too large to fit in memory at once. We show here our work on a Data Projector module that lets users arbitrarily cast multi-dimensional data into three spatial dimensions for visualization with a generic framework for interactive tuning and slicing of the other dimensions from the user interface. We will also discuss our recently released modular machine-learning segmentation engine called Segmentation Trainer and show how it is positioned to tightly integrate for advanced characterization of multi-modal and spectral datasets.
High-throughput instruments such as those at national laboratories can produce TB of experimental data a day, and it is increasing. However, the available software tools to organize and retrieve images cover a small fraction of our needs: “why do we continue using the umbrella-analogue solution to fight the data deluge?”

With the significant improvements in image processing speeds and availability of large storage systems, the development of methods to query and retrieve images is fundamental to support activities from simple human work with catalogues to complex research such as synthesizing new materials. These requirements motivated our team to develop pyCBIR, a new python tool for content-based image retrieval (CBIR) capable of searching relevant items in large databases, given unseen pictures. While much work in CBIR has targeted ads and recommendation systems, pyCBIR allows general-purpose investigation across image domains. Preliminary results indicate promising directions toward ranking X-ray scattering patterns from metallic crystal lattices. Currently, pyCBIR contains ten distance metrics, and six bags of features, including Convolutional Neural Networks implementations at a click-distance from users. We will also illustrate some of the applications of pyCBIR, from microCT screening to hypotheses generation using our inferential engine.
Workshop 2
Spectro-microscopy at the Nanoscale: Exploring Chemical, Electronic and Magnetic Properties of Novel Materials
May 15, 2017

**Location:** Bldg. 735, Center for Functional Nanomaterials (CFN), Large Conference Room

**Organizers:** Ruud Tromp, IBM T.J. Watson Research Center
Elio Vescovo, NSLS-II-BNL (vescovo@bnl.gov)
Jurek Sadowski, CFN-BNL (sadowski@bnl.gov)

**Description:** Synchrotron-based spectro-microscopies, such as x-ray photoemission electron microscopy (XPEEM) and high-resolution angle-resolved photoemission spectroscopy (ARPES) are powerful methods for studying chemical, electronic, and magnetic properties of materials. As new facilities, including the NSLS-II Electron Spectro-Microscopy (ESM) beamline, are coming online, they offer expanded capabilities for spectroscopic characterization of surfaces at nanometer scale. These new instruments and recent developments in k-space imaging/momentum microscopy generate increased interest in the science community. It opens new opportunities, but also creates new challenges in further technique development, as well as in the multi-dimensional, multi-set data acquisition and analysis. This workshop aims to bring together experts in the field of electron spectro-microscopy to explore these perspectives and challenges, spanning from new experimental capabilities for spectro-microscopic characterization of emerging materials, new spin filters and detectors, to the theory of electron optics.

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<th>Time</th>
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<td>8:30 a.m.</td>
<td><strong>Welcome</strong> (Continental Breakfast - included)</td>
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| 8:40 a.m. | **“New Frontiers for Spectromicroscopy with RIXS and ARPES”**
            L. Andrew Wray, New York University                                                   |
| 9:25 a.m. | **“ARI – a nano ARPES/ RIXS Facility at NSLS-II”**
            Konstantine Kaznatcheev, Brookhaven National Laboratory                              |
| 10:10 a.m. | Morning Break (included)                                                                   |
| 10:30 a.m. | **“ARPES at 120 nm: First Results of nanoARPES at the New MAESTRO Beamline at ALS”**
            Eli Rotenberg, Advanced Light Source                                                 |
| 11:15 a.m. | **“Measuring Electronic Structure in 4 Dimensions – a new Approach to Photoemission”**
            Gerd Schönhense, Univ. of Mainz, Germany                                               |
| 12:00 p.m. | Lunch (included)                                                                          |
| 1:00 p.m.  | **Tour of the Electron Spectro-Microscopy (ESM) Beamline**                                 |
| 2:00 p.m.  | **“A High Brightness Laser-based Light Source for Time-resolved Extreme Ultraviolet Photoemission Studies”**
            Thomas Allison, Stony Brook University                                               |
| 2:45 p.m.  | **“Spectroscopy with the Low Energy Electron Microscope”**
            Ruud Tromp, IBM T.J. Watson Research Center; Kamerlingh-Onnes Laboratory, Leiden Univ. |
| 3:30 p.m.  | Coffee Break (included) and Group Photo                                                   |
| 4:00 p.m.  | **“Ultrafast and Very Small: Discover Nanoscale Magnetism With Picosecond Time Resolution Using X-Rays”**
            Hendrik Ohldag, SLAC National Accelerator Laboratory                                 |
| 4:45 p.m.  | **“Magnetism at the Nanoscale Studied using X-PEEM at the Swiss Light”**
            Armin Kleibert, Paul Scherrer Insitut                                                 |
| 5:30 p.m.  | Workshop Adjourns                                                                         |
8:40 a.m.  
“New Frontiers for Spectromicroscopy with RIXS and ARPES”
L. Andrew Wray, New York University

New spectrographs promise to resolve RIXS and ARPES measurements on the sub-micron spatial scale, where mesoscale structure and quantum coherence can adopt new roles in the spectral function. I will review several specific scenarios in which these quasiparticle-resolving techniques can give incisive new information when applied as spectromicroscopy on important material systems such as battery electrodes and topological insulators.

9:25 a.m.  
“ARI – a nano ARPES/ RIXS facility at NSLS-II”
Konstantine Kaznatcheev, Brookhaven National Laboratory

High coherent flux, long experimental hall of NSLS-II source, for the first time, permit to combine full flux demanding near-Fermi edge spectroscopies, such as ARPES and RIXS with sub-100nm spatial resolution soft x-ray microscopy, a combination essential for study novel phenomena, where sensitivity and specificity of x-ray microscopy approaches the characteristic length and time scales of elemental excitation that define exceptional properties of quantum materials. Following presentation provides the technical description, expected capability and scientific goals of ARI (ARPES & RIXS nano-Imaging) beamline, accepted for construction at the NSLS-II, facility dedicated to the study of the nanoscale origin of macroscopic (electrical, magnetic and optical) properties of the matter, and the evolution of the system under relevant conditions.

10:30 a.m.  
“ARPES at 120 nm: First Results of nanoARPES at the New MAESTRO Beamline at ALS”
Eli Rotenberg, Advanced Light Source

In 2016, the new Microscopic and Electronic STRucture Observatory (MAESTRO) at the Advanced Light Source achieved first commissioning results. This experimental system fuses powerful sample preparation tools (glovebox, MBE, PLD) with state of the art photoemission end stations (μARPES, PEEM, nanoARPES) – all of which are connected through an automated UHV transfer system. A particularly novel feature of MAESTRO is its nanoARPES setup. This technique mates the merits of state of the art angle resolved photoemission (ARPES) with spatial resolution presently less than 120 nm, with an eventual goal of less than 50 nm, bringing k- and energy resolved electronic contrast on the nano- and mesoscale within reach. In this talk, we will present the key features of this machine and demonstrate its operation in two experimental showcases: data obtained on graphene sheets grown from SiC reveal fascinating landscapes of “volcanos” spitting out rivers of “carbon magma” at unprecedented resolution. Data on dichalcogenide WS2 nano-plates supported by TiO2 exhibit a wealth of detailed information on its chemical composition and band structure, and directly correlate to the spatially-dependent photoluminescence signal.

11:15 a.m.  
“Measuring Electronic Structure in 4 Dimensions – a new Approach to Photoemission”
Gerd Schönhense, Institute of Physics, Johannes Gutenberg University, Germany

The electronic structure of solids is a key element in materials research and –design. All transport and thermodynamical quantities of the electron system of a material depend on the Fermi surface and velocity vF; band dispersions determine optical and semiconducting properties. The method of choice to study the electronic structure is angular-resolved photoemission (ARPES), as described in textbooks (e.g. [1]). Here a new way to perform “multidimensional ARPES” (termed momentum microscopy) will be presented. High-resolution imaging of the Fourier plane of a cathode lens is combined with time-of-flight (ToF) energy recording, yielding maximal parallelization. The field of view in k-space exceeds the first Brillouin zone, the energy range comprises several eV. Tunable soft X-rays allow variation of the momentum component perpendicular to the surface via direct transitions to free-electron-like final states. This combination of concepts from microscopy and spectroscopy yields the 4D spectral density function p(E_F, k) (weighted by the photo-emission cross section), with ~10^8 resolved data points. Fermi surface and velocity distribution v_F(k_F) (see figure, from [2]), all band dispersions, electron or hole conductivity, effective mass and inner potential are obtained from p by simple algorithms. A set of apertures in an intermediate image plane allows precise definition of the region of interest down to ~1μm, independent on the footprint of the photon beam. An imaging spin filter gives access to the spin texture [3].
2:00 p.m.  “A High Brightness Laser-based Light Source for Time-resolved Extreme Ultraviolet Photoemission Studies”
Thomas Allison, Stony Brook University

Using high-power frequency comb methods, we generate femtosecond pulses of extreme ultraviolet (XUV) light at 87 MHz repetition rate and use these pulses for photoelectron spectroscopy experiments. With a compact XUV beamline, a single laser harmonic with < 50 meV bandwidth, ~100 fs pulses, and an average flux of more than 10^11 photons per second is delivered in a focused beam onto crystalline samples housed in a UHV surface science chamber. The photon energy is tunable between 10 and 40 eV in increments of 2.4 eV. With this high repetition rate, femtosecond time-resolved photoelectron spectra can be recorded from excited samples without the space charge effects that have plagued previous attempts at time-resolved XUV photoemission.

2:45 p.m.  “Spectroscopy with the Low Energy Electron Microscope”
Ruud M. Tromp, IBM T.J. Watson Research Center; Kamerlingh-Onnes Laboratory, Leiden University, Leiden, The Netherlands

The Photo Electron Emission Microscope (PEEM) and Low Energy Electron Microscope (LEEM) started out primarily as imaging instruments, just like the Transmission Electron Microscope (TEM). In recent years, however, PEEM and LEEM, while steadily improving imaging capabilities, have developed into powerful spectroscopic tools. While spatially-resolved Angle-Resolved Photo Electron Spectroscopy (ARPES) gives access to the occupied electron bands of a solid, Angle-Resolved Reflection Electron Spectroscopy (ARRES) reveals the unoccupied bands in 3D reciprocal space. Synchrotron-based core level spectroscopy gives chemical and magnetic information, surface plasmons can be seen with high time resolution with multi-photon laser-based PEEM, and with Electron Energy Loss Spectroscopy (EELS). Diffraction-based techniques allow for real-space potentiometry, as well as detailed growth and strain studies. Thus, LEEM/PEEM instruments bring together high resolution microscopy and a broad range of spectroscopic tools that have never been combined in a single instrument before. I will review state-of-the-art and outline directions for future development.

4:00 p.m.  “Ultrafast and Very Small: Discover Nanoscale Magnetism With Picosecond Time Resolution Using X-Rays”
Hendrik Ohldag, SLAC National Accelerator Laboratory

Today’s magnetic device technology is based on complex magnetic alloys or multilayers that are patterned at the nanoscale and operate at gigahertz frequencies. To better understand the behavior of such devices one needs an experimental approach that is capable of detecting magnetization with nanometer and picosecond sensitivity. In addition, since devices contain different magnetic elements, a technique is needed that provides element-specific information about not only ferromagnetic but antiferromagnetic materials as well. Synchrotron based X-ray microscopy provides exactly these capabilities because a synchrotron produces tunable and fully polarized X-rays with energies between several tens of electron volts up to tens of kiloelectron volts. The interaction of tunable X-rays with matter is element-specific, allowing us to separately address different elements in a device. The polarization dependence or dichroism of the X-ray interaction provides a path to measure a ferromagnetic moment and its orientation or determine the orientation of the spin axis in an antiferromagnet. The wavelength of X-rays is on the order of nanometers, which enables microscopy with nanometer spatial resolution. And finally, a synchrotron is a pulsed X-ray source, with a pulse length of tens of picoseconds, which enables us to study magnetization dynamics with a time resolution given by the X-ray pulse length in a pump-probe fashion.
Magnetism at the nanoscale is a vibrant research field in condensed matter physics, which is not only driven by the continuing demand for miniaturization of electronic and magnetic devices, but also by the unique properties and phenomena that emerge in nanomagnets due to spatial confinement and the high surface-to-volume ratio. At the surface/interface: microscopy (SIM) beamline at the Swiss Light Source (SLS) a broad research program that includes in-house and user projects benefits from the unique features of X-PEEM used together with X-ray magnetic circular dichroism (XMCD). The investigations span from molecular magnetism at interfaces to artificial spin ice systems and laser-induced magnetization dynamics. In this contribution, we will focus on our recent work on nanoparticle magnetism. For these investigations X-PEEM is combined with XMCD to investigate the magnetic properties of individual nanoparticles in large ensembles. Complementary scanning electron microscopy and atomic force microscopy investigations are used to correlate the magnetic properties of a large number of individual nanoparticles with their actual size and morphology. Using this unique approach we could directly demonstrate enhanced and metastable magnetism in individual, size- and shape-controlled 3d transition metal nanoparticles [1,2]. These findings not only help to clarify large discrepancies found in the literature on the magnetism of 3d transition metal nanoparticles, but provide also important insights to our understanding of the size-dependent evolution of magnetic properties in condensed matter. Moreover, our results may open new ways to tuning the properties of nanomagnets for applications.

Workshop 3  
Synchrotron Techniques in Support of DOE’s  
Subsurface R&D Effort  
May 15, 2017

Location: Bldg. 725, Computational Science, Seminar Room (2nd floor)

Organizers:  
Martin Schoonen, BNL (mschoonen@bnl.gov)  
Mohamed Elbakhshwan, BNL (bakhshwan@bnl.gov)  
Simerjeet K. Gill, BNL (gills@bnl.gov)  
Juergen Thieme, NSLS-II-BNL (thieme@bnl.gov)

Description: This proposed workshop will bring together several leaders of the multi-lab working group that developed the Subsurface R&D agenda, experts in the use of existing synchrotron facilities to study rocks and minerals, and experts in the development of new synchrotron facilities and techniques. The workshop will be initiated by short presentations on aspects of the Subsurface R&D agenda that can potentially benefit from synchrotron-based techniques. Examples of topics to be included in this introductory session are: 1) multi-phase flow in rock fractures; 2) mineral reactivity under subsurface conditions; 3) nanoporous rock structure, permeability and reactivity; 4) reactivity of mineral-brine-CO2 systems; and 5) alteration of cements and corrosion of casing under subsurface conditions. A second session will focus on promising synchrotron-based methods to address various aspects of the Subsurface R&D agenda. This includes the use of tomography on rock cores exposed to subsurface conditions; in operando structural deformation studies; and 3-D chemical imaging studies of geological materials, cements and steels. A third session will highlight the unique existing and future capabilities at NSLS-II. A final session will be a structured discussion to define future needs at NSLS-II to support research priorities of DOE’s Subsurface R&D effort.

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<td>8:40 a.m.</td>
<td>Continental Breakfast (included)</td>
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| 8:50 a.m. | Introduction and Welcome to the Workshop  
Mohamed Elbakhshwan, Brookhaven National Laboratory |
| 9:00 a.m. | “Brief Overview of DOE’s Subsurface Technology and Engineering Research, Development, and Demonstration (SubTER) Crosscut”  
Martin Schoonen, Brookhaven National Laboratory |
| 9:30 a.m. | “Atomic- to Pore-Scale Probes of Mineral Reactivity in Subsurface Environments”  
Andrew Stack, Oak Ridge National Laboratory |
| 10:00 a.m. | Morning Break (included) and Group Photo                            |
| 10:30 a.m. | “Mineral-Water Reactivity: Crossing the Interface”  
Paul Fenter, Argonne National Laboratory |
| 11:00 a.m. | “Frontier Areas in Mineral Interface Structure and Chemistry: Organics on Natural Surfaces; Grain Boundaries, and Nucleation Processes”  
Glenn Waychunas, Lawrence Berkeley National Laboratory |
|         | Subsurface Research Activities and the Cross Cutting Capabilities in Various DOE Laboratories (Open Discussion 1) |
| 12:30 p.m. | Lunch (included)                                                    |
| 2:00 p.m. | “Synchrotron Applications for Understanding Interfacial Redox Processes in Complex Geochemical Environments”  
Kevin Rosso, Pacific Northwest National Laboratory |
DOE has taken a leadership role in the science and technology for improved measurement, characterization, and understanding of subsurface environments with the goal of improving energy production as well as storage and management of energy waste streams. This effort is organized in a new interdisciplinary effort involving the DOE national laboratory complex and academia. The effort is organized around four broad research topics: 1) Wellbore Integrity & Drilling Technologies; 2) Subsurface Stress & Induced Seismicity; 3) Permeability Manipulation & Fluid Control; and New Subsurface Signals. This talk will highlight a few examples where existing or future synchrotron-based techniques might be used to support DOE’s SubTer Crosscut research agenda.

There is a strong need to develop a fundamental understanding of how mineral nucleation, growth and dissolution occur in porous media such as in the subsurface. The reason for this is two-fold, first, minerals can affect water quality by releasing or incorporating dissolved species, but also our ability to predict how porosity and permeability evolve with mineral reaction in response anthropogenic perturbation is limited. In this talk, I will show some of our recent work using X-ray and neutron scattering to examine how mineral reactions occur in porous media. This work is revealing some interesting questions about how the presence of the pores themselves affect the reactions, such the pore-size distribution in which precipitation preferentially occurs, or the rules governing phase selection. Especially important is when pore-size is reduced to length-scales on the order of some nanometers (i.e., nanopores), because a potentially different reactivity is introduced. These nanopores can constitute the majority of pores in some rock types such as shale, yet their reactivity and deviations from bulk-like behavior is not understood.

The mineral-water interface is a primary reaction site in low-temperature geochemistry. Yet our understanding of these systems is challenged by the need to make direct, in-situ, and real-time observations of these reactions. Over the past two decades, we have worked to observe the molecular-scale structure and dynamics at these interfaces, with an emphasis on the delineation of the “intrinsic complexity” of geochemical interface structure and reactivity, including changes to the mineral surface structure, the organization of interfacial hydration layers and the organization of ions at charged mineral-water interfaces. A new
challenge will be to extend this understanding to reactions that transcend isolated mineral-water interfaces to understand the additional roles of solution confinement and transport. To this end, we have begun to explore reactions at micron-scale mineral grains, with an initial emphasis on mineral-replacement reactions. Specifically, we have observed the replacement of micron-sized calcite ($\text{CaCO}_3$) grains by cerussite ($\text{PbCO}_3$) in acidic Pb-bearing solutions at room temperature. In spite of their differences in crystal structures (calcite vs. aragonite), the reaction proceeds through a dissolution reprecipitation reaction in which the formation of a cerussite shell around the calcite crystal is followed by further replacement of the calcite core.\(^1\) Calcite dissolution dominated the early stage of the reaction with the development of complex dissolution/growth features at the calcite surface that are controlled by the solution composition. The subsequent heterogeneous nucleation of cerussite nucleates heterogeneously suggesting that it is partially controlled by local supersaturation, and subsequent cerussite growth was influenced by the orientation of the synthetic calcite crystals with respect to the support. The results also revealed the presence of a fluid filled nano-pore layer (~150 nm) that was resolved between dissolving calcite and growing cerussite and appears to serve as a soft template for the pseudomorphic growth of cerussite.


11:00 a.m.  “Frontier Areas in Mineral Interface Structure and Chemistry: Organics on Natural Surfaces; Grain Boundaries, and Nucleation Processes”

Glenn Waychunas, Lawrence Berkeley National Laboratory

The subsurface is a complex geochemical structure containing not only mineral grains but many types of organic molecules, living cells and both organic-rich and aqueous-rich fluids. All of these react with one another at fluid-mineral interfaces. Most current experiments are reductionist and deal with simple surfaces, or very simple chemistry. However to make sense of subsurface processes ultimately we need to both describe and model realistic aspects of these structures and components. Organics at interfaces are presently being studied in a variety of ways using synchrotron techniques, but progress may depend on the use of laboratory-based instrumentation in synchrony with synchrotron light. Work using organic components in fluids, or coexisting fluids and vapors may profitably be studied using synchrotron-based IR probes, while analogous AFM-based near-field IR instruments may allow complex interfacial organic structures to be probed.

A large unknown area is the structure and composition of grain boundaries both in “solid” rocks and in sediments. The scales involved are small enough so that information on the phases present and their locus remains limited, but nanometer methods (x-ray nanoprobe spectrometry and spectroscopy, near field IR spectroscopy and ptychography) can extend knowledge dramatically. In particular, grain boundary characterization may lead to improved knowledge of how rocks fail, either by natural or technological processes. For grains in near surface rocks or sediment units, the nature of grain boundaries may be critical to understanding transport and retention of both toxins and nutrients in the environment.

Carbonate nucleation reactions are being studied in detail with respect to carbon sequestration concepts, using GISAXS methodologies. But nucleation processes in many other systems are not well understood. The formation of iron oxyhydroxides is a case in point. For this system synchrotron time-resolved EXAFS, and PDF analysis have been very helpful. Use of synchrotron and FEL-based pulse structure may also allow nucleation (and other) processes to be decomposed and their transition states resolved.

2:00 p.m.  “Synchrotron Applications for Understanding Interfacial Redox Processes in Complex Geochemical Environments”

Kevin Rosso, Pacific Northwest National Laboratory

Research in new energy systems development critically depends on understanding geochemical processes in the deep subsurface, both for resource extraction and waste disposal. To make fundamental advances requires robust experimental and computational approaches to unravel rate controlling factors at mineral/water interfaces at the atomic scale. This presentation will overview current use and emerging needs for synchrotron-based absorption and scattering spectroscopies applied to a variety of interfacial redox processes, emphasizing the multi-disciplinary complex problem
of aqueous Fe(II)/Fe(III)-oxide interaction. At redox gradients in natural waters, as well as in corrosion fronts in metals, changes in the electrochemical potential impact iron valence distribution, and, in turn, phase stabilities and aqueous solubilities. In almost all cases, aqueous Fe(II) is juxtaposed against sparingly soluble Fe(III) solids. Highly soluble Fe(II) catalyzes recrystallization of hydrous ferric oxides into more crystalline and stable Fe(III)-oxyhydroxides and oxides. Beyond very informative high resolution electron and atomic force microscopies, synchrotron X-ray absorption and scattering analyses along with isotopically labelled Fe tracer studies show that recrystallization is facile and involves a moving front through solid interiors. Polaronic electron mobility through these solids appears to play a key role, linking spatially remote interfacial ET donor and acceptor site across nanophase crystallites, and defining the activation energy for redox reactions. Crystal truncation rod X-ray scattering of the Fe-oxide/water interface shows the importance of adsorbed water organization and dynamics on interfacial structure. Ambient pressure X-ray photoelectron spectroscopy is enabling exploration of interfacial structure as a function of water chemical potential. Fe L-edge X-ray magnetic circular dichroism is helping unravel interfacial structure in terms of both Fe valence and local coordination. From the combined techniques the critical roles of bulk and interfacial structural defects on the rates of redox processes can be clearly identified. The approaches seem well poised to enable significant new insights into factors controlling interfacial redox dynamics generally, and help lay out a path for resolving a wide range of challenging interfacial geochemistry topics in the future.

2:30 p.m.  “Synchrotron Techniques in Support of Sustainable Subsurface Energy Technologies”
Catherine A. Peters and Jeffrey P. Fitts
Department of Civil & Environmental Engineering, Princeton University
cap@princeton.edu

Numerous synchrotron techniques provide valuable information about rock structure, spatial distributions of minerals, and composition of mineral precipitates. Such information is critical to understanding thermodynamic and kinetic processes relevant to geochemical processes of the subsurface. Geochemical processes play an important role in the context of subsurface energy technologies including geologic carbon sequestration, geothermal energy production, deep borehole nuclear waste disposal, subsurface energy storage, etc. For example, acid-driven dissolution of carbonate minerals can increase fracture permeability, and in the context of geologic carbon sequestration this could jeopardize storage security. Geochemical processes are also important in sustainable management of flowback and produced waters in oil & gas operations. For example, addition of sodium sulfate can be added to induce precipitation of the sparingly soluble mineral barite (barium sulfate), which fortuitously co-precipitates toxic trace elements like Radium and Arsenic.

This presentation includes an overview of synchrotron techniques that have been used in Dr. Peters’ research to elucidate mineral spatial patterns and void space in fractured and porous media. The following examples will be presented. (1) X-ray computed tomography for 3D characterization of rock fracture geometry and its evolution in reactive flows. (2) X-ray attenuation to measure fracture surface geometry changes in 2D. (3) X-ray computed tomography to reveal microscopic pore structure evolution caused by calcite depletion. (4) X-ray computed tomography to generate 3D maps of mineral distributions in shales. (5) Micro XRF and micro XRD imaging to generate 2D maps of reactive minerals on fracture surfaces. (6) X-ray nanoprobe imaging of co-precipitated substances in barite nanoparticles.

3:30 p.m.  “Unraveling Structure and Performance of Subsurface Materials using High Resolution Synchrotron Methods”
Simerjeet Gill, Brookhaven National Laboratory

High resolution synchrotron methods offer an excellent opportunity to gain fundamental understanding of kinetics and reaction mechanisms that occur at solid-fluid and solid-solid interfaces under extreme conditions of temperature, pressure and corrosive environments present in various energy systems, such as subsurface and enhanced geothermal systems. The dissolution and precipitation reactions that occur at solid-fluid (cement-fluid) interfaces under hydrothermal conditions as well as carbon sequestration need to be understood as they can lead to drastic loss in permeability, which may limit the economic viability of sequestration. Also, in the oil, gas, and geothermal energy fields, fundamental understanding of the interfacial bonding at solid-solid interfaces (cement-casing) is lacking; which is critical for complete and durable zonal
isolation. Such knowledge will not only help predict economic viability of sequestration and well integrity but will also help in designing next generation materials with enhanced performance under extreme geothermal conditions.

In our approach, we utilize high resolution and ultra-fast X-ray based synchrotron methods to study microstructure and interfacial interactions at cement-fluid and cement-casing interfaces. Solid-fluid interactions, in well and advanced polymer based cements and solid-solid interactions in cement-casing interfaces under geologic sequestration and hydrothermal conditions, elucidated using x-ray based synchrotron methods will be discussed. In addition, the elemental, chemical and microstructural changes using X-ray fluorescence (XRF) and X-ray absorption near edge structure spectroscopy (XANES) and computed tomography (CT) in advanced cements and cement-casing interfaces after exposure to corrosive environments will be discussed.

4:00 p.m.  “Microprobe Spectroscopy at the 5-ID Beamline of NSLS-II”
Garth Williams, Brookhaven National Laboratory

The sub-micron resolution x-ray spectroscopy (SRX) beamline leverages the extremely stable source provided by NSLS-II to probe the composition and chemical state of matter at specific locations within the sample. The most commonly used configuration of the instrument uses long-working distance x-ray focusing mirrors to create a sub-micron x-ray spot; however, smaller focal spots and limited full field imaging capabilities are planned for the future. The energy of this beam is tunable in the range 4-25 keV, allowing micro-spectroscopic studies on elements ranging from Ti to Pt. The long working distance permits the use of novel sample cells, for example, to hold the sample at cryogenic, or elevated, temperatures or monitor electrochemical changes. We will introduce the capabilities of SRX and provide examples highlighting these.
Workshop 4  
Measurement and Interpretation of Diffuse Scattering in X-Ray Diffraction for Macromolecular Crystallography  
May 15, 2017

**Location:**  Bldg. 555, Chemistry Department, Hamilton Seminar Room

**Organizers:**  
Robert Sweet, NSLS-II-BNL (rsweet@bnl.gov)  
Michael Wall, Los Alamos National Laboratory (mewall@lanl.gov)  
Nozomi Ando, Princeton University (nozomi.ando@princeton.edu)  
James S. Fraser, University of California, San Francisco (jfraser@fraserlab.com)  
George N. Phillips, Jr., Rice University (georgep@rice.edu)

**Description:** X-ray diffraction from macromolecular crystals includes both sharply peaked Bragg reflections and diffuse intensity between the peaks. The information in Bragg scattering reflects the mean electron density in the unit cells of the crystal. The diffuse scattering arises from correlations in the variations of electron density that may occur from one unit cell to another, and therefore contains information about collective motions in proteins. A major focus of the workshop will be to provide a roadmap to the acquisition of reliable data by surveying measurement methods and discussing the increase in measurement accuracy enabled by improved detectors, experimental methods, and data integration. Missing from recent results is real information about the behavior of the molecules being studied that would guide the thinking of biochemists and biologists. To discuss these and their relative merits will be a second major focus of the workshop. The charge to this workshop will be to provide a roadmap to efforts that will provide the biological understanding we believe is hidden in the data.

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<tr>
<th>Time</th>
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<tr>
<td>8:30 a.m.</td>
<td>Continental Breakfast (included)</td>
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| 8:30 a.m. | Welcome, Introduction, and Charge to the Workshop  
Robert Sweet, Brookhaven National Laboratory |
| **Session 1** |                                                                                          |
| 8:40 a.m. | “Measuring and Modeling Diffuse Scattering in MX Diffraction Patterns”  
Michael Wall, Los Alamos National Laboratory |
| 9:10 a.m. | “General Principles of Protein Diffuse Scattering with Some Examples”  
George Phillips, Rice University |
| 9:40 a.m. | “Experimental Approaches to Diffuse Scattering from Solution X-ray Scattering”  
Nozomi Ando, Princeton University |
| 10:10 a.m. | Morning Break (included) and Group Photo                                                         |
| 10:30 a.m. | “Early Studies in the Discipline”  
Donald Caspar, Florida State University |
| 11:00 a.m. | “Observations from the Ribosome on a Source of Diffuse Scattering”  
Peter Moore, Yale University |
| 11:30 a.m. | “Insights from Total Scattering Simulations”  
James Holton, Lawrence Berkeley National Laboratory |
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<th>Time</th>
<th>Session 2</th>
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<tr>
<td>12:00 p.m.</td>
<td>Lunch (included)</td>
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<tr>
<td>12:45 p.m.</td>
<td>“Properties and Analysis of Continuous Diffraction of Disordered Crystals”</td>
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<td>Henry Chapman, Deutsches Elektronen-Synchrotron</td>
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<tr>
<td>1:15 p.m.</td>
<td>“Ultra-low Background Graphene Microfluidics”</td>
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<td>Sarah Perry, University of Massachusetts, Amherst</td>
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<tr>
<td>1:45 p.m.</td>
<td>Extracting Diffuse Data from X-ray Diffraction Patterns # 1</td>
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<td>Mitchel Miller, Rice University</td>
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<tr>
<td>2:00 p.m.</td>
<td>Extracting Diffuse Data from X-ray Diffraction Patterns # 2</td>
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<td>Alexander Wolff, University of California, San Francisco</td>
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<tr>
<td>2:15 p.m.</td>
<td>“Reflections on Integrating Bragg Spots in Serial Crystallography”</td>
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<td>Nicholas Sauter, Lawrence Berkeley National Laboratory</td>
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<tr>
<td>2:45 p.m.</td>
<td>Coffee Break (included)</td>
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<tr>
<td>3:00 p.m.</td>
<td>“Birth of the Cool: Multitemperature Multiconformer X-Ray Crystallography”</td>
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<td>James Fraser, University of California, San Francisco</td>
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<tr>
<td>3:30 p.m.</td>
<td>“Molecular Dynamics Simulations of Protein Crystals”</td>
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<td>David Case, Rutgers University</td>
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<tr>
<td>4:00 p.m.</td>
<td>“Hybrid Methods for Modeling the Protein Conformational Ensemble using X-ray Crystallography”</td>
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<td>Henry van den Bedem, Stanford Synchrotron Radiation Lightsource</td>
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<tr>
<td>4:30 p.m.</td>
<td>Discussion</td>
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<tr>
<td>5:30 p.m.</td>
<td>Workshop Adjourns</td>
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# Workshop 5
## Bringing Big Science into the Classroom
### May 17, 2017

**Location:** Bldg. 725, Computational Science, Seminar Room (2nd floor)

**Organizers:**
- Alida Perez, OEP-BNL (pereza@bnl.gov)
- Lisa Miller, NSLS-II-BNL (lmiller@bnl.gov)
- Fernando Camino, CFN-BNL (fcamino@bnl.gov)

**Description:** Every high school science teacher will tell you that students usually learn science best in the laboratory, recreating the experiments that defined modern scientific discovery and theory. Unfortunately, many of the most interesting experiments require instrumentation and equipment that is simply too costly for a classroom laboratory. This session is designed to provide participants the opportunity to learn about two premier research facilities at BNL, the National Synchrotron Light Source II (NSLS-II) and the Center for Functional Nanomaterials (CFN), as resources for the high school science classroom. Participants will learn how teachers and their students become users of these facilities, allowing them to go beyond classroom walls to utilize unique research tools, the same used by Nobel Prize winning scientists. Participants will also learn how to gain remote access to NSLS-II and CFN via internet-enabled tools, allowing students to answer real scientific questions from their classroom laboratory. In addition, session presenters will include teachers that are facility users and will share their experiences and students’ research outcomes. This workshop will be offered free of charge to participants through the generous sponsorship from the NSLS-II and CFN UECs.

Roundtable Discussion Moderators: Robert Bolen, Maria Brown, Lora Hine, Tony Lanzilotti (University of Chicago), Tracy Walker (Canadian Light Source), Dan Williams.

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<tr>
<td>8:45 a.m.</td>
<td>Continental Breakfast (included)</td>
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<td>9:00 a.m.</td>
<td><strong>Welcoming Remarks</strong></td>
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<td>Chuck Black and Qun Shen, CFN / NSLS-II, Brookhaven National Laboratory</td>
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<td>9:30 a.m.</td>
<td><strong>“Introduction to NSLS-II and Student Research Opportunities”</strong></td>
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<td>Lisa Miller, Brookhaven National Laboratory</td>
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<tr>
<td>9:55 a.m.</td>
<td><strong>“Shaping the Scientific Workforce of the Future: A Partnership of Long Island High Schools and a World-Class Nanoscience Facility”</strong></td>
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<td>Fernando Camino, Brookhaven National Laboratory</td>
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<tr>
<td>10:20 a.m.</td>
<td>Morning Break (included)</td>
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<td>10:30 a.m.</td>
<td><strong>“An Overview of Educational Initiatives at NSLS and APS”</strong></td>
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<td>Tony Lanzilotti, University of Chicago</td>
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<tr>
<td>11:00 a.m.</td>
<td><strong>“Inspiring Young Scientist to Accelerate using Illumination”</strong></td>
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<td>Mary Kroll, West Islip School District</td>
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<td>11:40 a.m.</td>
<td><strong>“CFN Introduces Nanotechnology in Freeport’s District K-12 Science Curriculum”</strong></td>
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<td>Edward Irwin, Freeport Public Schools</td>
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<tr>
<td>12:20 p.m.</td>
<td>Lunch (included)</td>
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<td>1:00 p.m.</td>
<td><strong>“The NISE Network: Engaging the Public, Leveraging Partnerships, Building Capacity”</strong></td>
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<td>Emily Cotman, NISE Net</td>
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1:30 p.m.  “Xraise: Shedding New Light on K-12 Educational Programs”
           Lora Hine, Cornell High Energy Synchrotron Source

2:00 p.m.  Round Table Discussion

2:45 p.m.  Coffee Break (included) and Group Photo

3:00 p.m.  Facilities Visit: NSLS-II and CFN

5:00 p.m.  Workshop Adjourns

9:30 a.m.  “Introduction to NSLS-II and Student Research Opportunities”
           Lisa Miller, Brookhaven National Laboratory

As a National User Facility operated by the US Department of Energy, one of the missions of NSLS-II is to train the next generation of scientists by providing them with the opportunity to formulate a hypothesis-driven scientific problem and use a world-class facility to conduct their research. In this talk, I will provide an overview of the NSLS-II facility and some of the current beamline techniques and capabilities that are available for student research projects. I will also describe the proposal process for accessing the facility and provide some examples of past projects.

9:55 a.m.  “Shaping the Scientific Workforce of the Future: A Partnership of Long Island High Schools and a World-Class Nanoscience Facility”
           Fernando Camino, Brookhaven National Laboratory

An essential part of the DOE science mission is developing the nation’s scientific workforce of the future — a mission the Center for Functional Nanomaterials supports by engaging students at all levels, exposing them to a world-class nanoscience research facility, and inspiring them with the exciting work that we do. In this talk, I will provide an overview of the outstanding nanoscience carried out at our Center, and describe innovative examples illustrating our commitment to workforce development. I will suggest that there are exciting new ways for the CFN to interact with young students interested in science, including on projects preparing new science modules for the annual community Summer Sunday open house. Another possibility is implementing a student-targeted nanoscience colloquium, whose content can be pre-discussed in the classroom, so that students are better equipped to learn the topic and formulate questions.

10:30 a.m.  “An Overview of Educational Initiatives at NSLS and APS”
           Tony Lanzirotti, University of Chicago

In this talk, I will discuss his involvement in the development of education programs at the National Synchrotron Light Source and at the Advanced Photon Source to provide 7-12th grade science teachers and their students the experience of conducting scientific experiments at two of the premier User Facilities in the United States. Both programs were developed to provide educators and students an opportunity to conduct original research using synchrotron radiation, primarily engaging these student groups to try and formulate innovative research questions on their own rather than trying to simply reproduce experiments done by others. I will provide an overview of both programs and discuss the goals that were set forth when they were developed and the lessons learned. I will also provide examples of some of the research participating groups have come up with. In some cases, the research is surprisingly competitive with studies proposed by many general users that apply for beamtime.

11:00 a.m.  “Inspiring Young Scientist to Accelerate using Illumination”
           Mary Kroll, West Islip School District

A workforce evolution is well underway with science and technology playing crucial roles in all avenues of progression. The result is an urgency to prepare our students for careers in these fields. Increasing exposure
Agendas

and experiences using advanced scientific tools and techniques to solve problems are key to inspiring future scientists. Becoming a teacher user at the NSLS-II in order to bring this cutting edge technology into the classroom is a worthwhile undertaking and not as daunting as one may presume. The result is real science being done in your classroom using data generated by technology that will excite your students. With web conferencing and remote access, large numbers of students can actually utilize advanced research tools that previously could only be taught using photos and stories. The scientists and staff at Brookhaven National Laboratory and the NSLS-II are ready and willing to help you brighten your science curricula and inspire your students to consider careers in science and technology.

11:40 a.m.  “CFN Introduces Nanotechnology in Freeport’s District K-12 Science Curriculum”
Edward Irwin, Freeport Public Schools

The science research program at Freeport High School is based on an educational model where students receive a strong foundation in the basic tenets of scientific method and laboratory skills tailored to the specific interests of the student. More specifically, students are taught research design and hypothesis testing methods, as well as a broad range of laboratory skills including molecular biology, animal models, microscopy, and physics. The research program is open to all students and they are required to submit their own independent research project. This strong foundation in scientific research is gained through work done on location at Freeport High School with the goal of preparing students for immediate transition to academic productivity when joining a laboratory after graduation during their undergraduate education and beyond. Partnership with the Brookhaven National Laboratory’s Center for Functional Nanoparticles and the National Synchrotron Light Source programs have provided a unique opportunity for Freeport students to transition to an outside laboratory prior to graduation and further expand their research skills. The students have been able to work in a high-level academic setting with mentorship from leading scientists using state-of-the-art equipment, including electron microscopes and instruments for spectral analysis. Both in-person and video-teleconference meetings provide an extension for the work done at Brookhaven Labs, where students have direct access to scientists for guidance and feedback on their projects. This model of scientific education, made possible through partnership with Brookhaven National Laboratory, provides a pathway for accelerated scientific training for the next generation of scientists and the New York State School Boards Association, 2016 Be The Change For Kids Award for our nanotechnology curriculum. The culmination of these efforts have resulted in Freeport students continuing scientific research at the country’s top Universities including MIT, Cornell, Columbia and New York University.

1:00 p.m.  “The NISE Network: Engaging the Public, Leveraging Partnerships, Building Capacity”
Emily Cotman, NISE Net

Over ten years, the Nanoscale Informal Science Education Network (NISE Net) created a national community of researchers and informal science educators dedicated to fostering public awareness, engagement, and understanding of nanoscale science, engineering, and technology. NISE Net includes more than 600 museums, universities, and other organizations. Network partners work together to engage the public in learning about current science, engineering, and technology. Collectively, our efforts give the Network broad reach to diverse public audiences across the United States.

NISE Net has created widespread motivation and capacity to engage public audiences in current science and emerging technologies. In 2016, NISE Net transitioned to an ongoing identity as the National Informal STEM Education Network, leveraging the investment of the National Science Foundation for new projects and collaborations. The National Informal STEM Education Network brings together educators, scientists and engineers, and diverse public audiences to talk and learn about a wide range of STEM topics. Learn more at www.nisenet.org.
Xraise, the education and public outreach arm of the Cornell High Energy Synchrotron Source, offers innovative educational experiences for hundreds of precollege participants each year. Xraise engages minds by facilitating direct interactions with physical phenomena and encouraging careful observation of the world. These direct experiences consist of hands-on explorations that embrace the same processes that experts practice at our world-class laboratory.

The Xraise team will share several examples of learning activities developed for high school, illustrating the capabilities of synchrotron science and connecting students’ existing science knowledge to real-world applications. Presentation highlights include a diffraction demonstration from our High School Lending Library collection; an illustration of our portable X-ray fluorescence (XRF) equipment and corresponding learning opportunities for educators and students; and the exhibition of the Junk Genies of Science project, interactive exhibits built by students to illuminate synchrotron science concepts. Lively discussion is strongly encouraged!
Workshop 6
Polarized Resonant Soft X-ray Scattering at the NSLS-II
May 17, 2017

Location: Bldg. 488, Berkner Hall, Conference Room B

Organizers: Eliot Gann, NIST (eliot.gann@nist.gov)
Dan Fischer, NIST (dfischer@bnl.gov)
Dean DeLongchamp, NIST (dean.delongchamp@nist.gov)

Description: Polarized Resonant Soft X-ray Scattering is an exciting new capability which will soon be coming to NSLS-II. NIST has secured funding to build an P/RSoXS station as part of NIST’s suite of beamlines (at SST). RSoXS provides a few key advantages over more established hard X-ray scattering. In particular the use of energies between 100-2000 eV allows probing of K and L edges of many low-z materials which have exceedingly low contrast at higher energies. Thin film relevant systems with thicknesses of several to several hundred nanometers can be examined, while a continually variable contrast can pick out material-specific morphology. It will be vitally important to get some key current and potential users of the technique together to discuss the early successes and areas for expansion particularly new sample environments and the detailed use of polarization dependence. Particular focus will be on areas where a new beamline can expand upon the capabilities of existing facilities.

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<tr>
<td>8:30 a.m.</td>
<td>Continental Breakfast (included)</td>
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<tr>
<td>8:30 a.m.</td>
<td>Welcoming Remarks and Beamline Design Overview</td>
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<td>Eliot Gann, Dean DeLongchamp and Dan Fischer, BNL/NIST</td>
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<tr>
<td>8:40 a.m.</td>
<td>“Multimodal Resonant X-ray Scattering for Energy Materials at ALS”</td>
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<td>Cheng Wang, Advanced Light Source</td>
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<td>8:55 a.m.</td>
<td>“Using Manufacturing Customers to Drive Innovation, Impact, and Funding of Neutron and X-ray User Facilities”</td>
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<td>Ronald Jones, National Institute of Standards &amp; Technology</td>
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<td>9:10 a.m.</td>
<td>“Critical Factors that Affect Complex Morphology and Performance Metrics in High-efficiency Nonfullerene Organic Solar Cells”</td>
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<td>Long Ye, North Carolina State University</td>
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<td>9:25 a.m.</td>
<td>“Understanding Electrical Conductivity in Semiconducting Polymers through Resonant Soft X-ray Scattering”</td>
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<td>Eunhee Lim, University of California at Santa Barbara</td>
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<td>9:40 a.m.</td>
<td>“Resonant Soft X-ray Scattering of Biological Systems”</td>
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<td>Enrique Gomez, Penn State University</td>
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<td>Brian Collins, Washington State University</td>
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<td>10:10 a.m.</td>
<td>Coffee Break (included) and Group Photo</td>
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<td>10:40 a.m.</td>
<td>“Oxygen K Edge Scattering from Bulk Comb Diblock Copolymer: Extended, Ordered Backbones above the Lamellar Order-Disorder Transition”</td>
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<td>Jeffrey Kortright, Lawrence Berkeley National Laboratory</td>
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<td>10:55 a.m.</td>
<td>“Strategies for Multi-Modal Analysis”</td>
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<td>Alexander Hexemer, Lawrence Berkeley National Laboratory</td>
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### 8:40 a.m. **“Multimodal Resonant X-ray Scattering for Energy Materials at ALS”**  
Cheng Wang, Advanced Light Source, Lawrence Berkeley National Laboratory

Recent development of resonant soft x-ray scattering (RSoXS) at the Advanced Light Source (ALS) has enabled its applications to many critical research areas of materials research. Combining conventional x-ray scattering with soft x-ray absorption spectroscopy, RSoXS is a unique chemical sensitive structure probe that provides a novel route to unambiguously decipher the complex morphologies of mesoscale materials. Tuning x-ray photon energies to match the absorption spectrum of the different chemical components, the scattering contributions from the different components can be selectively enhanced, enabling a glimpse into these complex morphologies with unprecedented details. Applications of RSoXS have been extended to the areas of structured polymer assemblies, organic electronics, functional nano-composites, as well as liquid crystals.

The overarching challenge now across various disciplines is to investigate the interfacial phenomenon of new and complex materials in their operational conditions, including batteries, catalysts, gas separations, fuel cells and water desalination, and bio-hybrid systems. In order to achieve comprehensive understanding of the in-operando process, we need multimodal research tools that provide information from different perspectives in order to discover, understand, and control the interfacial phenomena and architectures. This will require combining different in situ probes, such as x-ray scattering and electron microscopy, simultaneously in the same operating condition. We will discuss the recent development of customized instrumentation, multimodal characterization methods, as well as comprehensive theory for the extraction of the chemical distribution and spatial arrangement at multiple length scales in the application of energy materials.

### 8:55 a.m. **“Using Manufacturing Customers to Drive Innovation, Impact, and Funding of Neutron and X-ray User Facilities”**  
Ronald Jones, National Institute of Standards & Technology

The emergence of Soft X-rays as a cutting edge probe of materials at all lengths scales promises to revolutionize the fundamental understanding of material structure while also answering critical questions in manufacturing. As such, it is key that we make the connections at the onset between efforts at national laboratories between instrument developers, user communities, and the manufacturing sectors that will reap the most benefit from these techniques. Bringing these communities together now will pay dividends through the enhancement of impact of the measurements and alignment of instrument evolution with the needs landscape of materials discovery and manufacturing. As an example, I will highlight the development of an industrial consortium, nSoft, formed in the fall of 2012 to create a path for manufacturers of soft materials to learn about and access neutron resources and NIST staff working in key areas of technology for this sector. nSoft continues to grow into new arenas and has proven an effective collaboration mechanism in a non-proprietary environment. I will briefly describe the consortium, and highlight how member companies and NIST staff are leveraging the consortium successfully to make real impacts in their research and development, both in a fundamental and applied sense. As the consortium grows, member companies have increased their investment in nSoft by a factor of 2 each year, allowing NIST staff to pursue increasingly bold ideas for instrument development and scientific pursuit. I will also highlight problems where I believe soft X-rays can provide immediate and more long term impact in these types of collaborations, again focusing on soft materials manufacturers.
9:10 a.m.  “Critical Factors that Affect Complex Morphology and Performance Metrics in High-efficiency Nonfullerene Organic Solar Cells”
Long Ye¹*, Sunsun Li², Subhrangsu Mukherjee¹, Jianhui Hou², Harald Ade¹
¹ Department of Physics, North Carolina State University, Raleigh, NC 27695, USA
² Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China  *E-mail: lye4@ncsu.edu

In the organic photovoltaics field, currently available polymer acceptors along with hundreds of novel nonfullerene acceptors create an incredibly large pool of polymer:acceptor pairs that would be difficult to optimize without a complete characterization and fundamental understanding of the complex and often multi-length scale morphology. Our recent demonstration[1] of 12%-efficiency in fullerene-free organic solar cells brings many questions critical to the operation of these novel organic devices into focus: What are the critical factors that affect the complex morphology of nonfullerene solar cells? Through detailed characterizations (hard/soft X-ray scattering), we show that a linear correlation between the average purity variations at the smallest length scale (~10 nm) and photovoltaic device characteristics across all processing protocols in ~12%-efficiency nonfullerene material systems[2]. This correlation is indeed universal for organic solar cells with multi-length scale morphology, irrespective of acceptor materials used (fullerenes, nonfullerene molecular acceptor, or conjugated polymers)[2-4] and fabrication methods used (spin-coating or blade-coating)[5]. Moreover, we also find high volume fraction or average purity of smallest domains is a critical requirement for high efficiency printed nonfullerene organic solar cells.

References

9:25 a.m.  “Understanding Electrical Conductivity in Semiconducting Polymers through Resonant Soft X-ray Scattering”
Eunhee Lim, University of California at Santa Barbara

Organic semiconductors provide a unique opportunity for developing large area, flexible electronics such as solar cells, displays, and wearable electronics. In order to better understand the performance of electronic devices, there has been significant progress in studying the structure – property relationship of organic semiconductors. The morphology of the semiconductors over large length scales can be controlled by molecular design and processing methods to achieve improved performance of organic semiconductors.

Enhancing the electrical conductivity of semiconducting polymers through chemical doping has been of great interest for many applications in organic electronics including electrode layers and thermoelectric devices. Finding an efficient doping method is important as doping methods in thin films affect the film morphology, which is closely related to charge transfer and transport.

Resonant soft X-ray scattering (RSoXS) is a unique tool with high chemical and bond orientation sensitivity that can be used to probe both crystalline and amorphous regions in organic thin films. By employing RSoXS, we study the orientation correlation length (OCL) of polymer backbone in thin films and show how the OCL correlates with conductivity in doped semiconducting polymers. With better understanding of the impact of doping on morphology and electrical properties, we can continue to improve performance of organic semiconductors.
The structure at one to a few hundred nanometers is critical to the properties and functionality of proteins, lipid membranes, hydrogels and a variety of complex biological assemblies. Small angle X-ray scattering is a powerful tool capable of probing the aforementioned length scales, but is often limited by the relatively small differences in electron density between phases or domains of soft materials. Resonant soft X-ray scattering (RSoXS), a technique developed within the last decade for the study of polymeric thin films, couples spectroscopy and scattering to overcome some of the critical limitations of hard X-ray scattering. Conventional X-ray scattering relies on circa 8 keV X-rays as the incident radiation; in contrast, RSoXS employs X-ray energies between 0.2 and 1.5 keV to access various absorption edges (e.g., C, N, O, F, Ca) and enhance scattering contrast. Working at these lower energies, however, requires a high-vacuum sample chamber. We have been taking advantage of recent advances in wet-cell technology for transmission electron microscopy experiments to enable RSoXS of biological materials in solution, thereby opening the door for extracting chemical contrast from multicomponent biological assemblies. We have demonstrated proof-of-concept experiments using wet-cell RSoXS to extract the envelope function of proteins. Furthermore, we have used RSoXS to examine the structure of plant cell walls, where we extract the average spacing between cellulose nanofibrils.

Carbon based (organic) materials embody a revolution in technology, being printable, flexible, and biocompatible. Internal nanostructure – especially at interfaces – often determines their mechanical, optical, and electronic properties but has been exceedingly difficult to probe. Recently bond-sensitive resonant soft X-ray scattering (RSoXS) has shown promise in revealing these critical structures. Through the intrinsic capability to tune contrast via photon energy, RSoXS provides an extra dimension of information above traditional scattering techniques. To take maximum advantage of this information, we have developed optical scattering models that can quantitatively separate different structures or types of ordering within one sample. We apply this model to block copolymer thin films and show how it can be used to measure quantitative details of the interface between the blocks – information critical to both polymer physics and photolithography applications. The model is extended to polymer-fullerene blends of interest to organic electronics research. As this tool is more fully developed, RSoXS will become central for revealing the most hidden scientific answers, enabling the next generation materials and technologies.

The evolution of molecular morphology in bulk samples of comb diblock copolymer pNdc,12-b-pNte,21 across the lamellar order-disorder transition (ODT) is studied using oxygen K edge scattering to determine whether the molecules remain extended or collapse above the ODT. The distinct spectral resonances of carbonyl oxygen on the backbone and ether oxygen in the pNte side chains combine with their different site symmetry within the molecule to yield strong differences in structural sensitivity at all temperatures. Comparison with simple models for the disordered phase reveals that disordering at the ODT corresponds to loss of positional order of molecules with extended backbones that retain orientational order, rather than backbone collapse into a locally isotropic disordered phase. This conclusion is facilitated by the distinct structural sensitivity at the two resonances. The roles of depolarized scattering in enhancing this sensitivity, and background fluorescence in limiting dynamic range, in oxygen resonant scattering are discussed, as are implications for improved RSoXS instrumentation.
11:10 a.m.  "Resonant Soft X-ray Scattering for Block Copolymer Lithography"
Joseph Kline, National Institute of Standards & Technology

The semiconductor industry continues to produce ever smaller nanodevices to power the latest integrated circuits. The small dimensions are reaching the fundamental limits of current optical lithography methods. New methods such as EUV lithography and directed self assembly (DSA) are being developed to pattern the smaller dimensions needed for next generation devices. DSA is used to drive the orientation of the self assembly of block copolymers. DSA is a combination of bottom-up and top-down lithography. The smallest dimensions are determined synthetically through the molecular length of the blocks in the copolymer and the placement and long range arrangement are from guide structures patterned by conventional lithography. One of the key challenges of DSA is characterization of the arrangement of the two blocks. The polymers frequently have similar density and thus small scattering contrast. Soft X-rays allow contrast based on the functional groups in the two polymer blocks. Variable angle transmission soft X-ray scattering was used to measure the “single crystal” diffraction from a periodic nanostructure consisting of the block copolymer pattern. Fitting the scattering pattern allows determination of the size and shape of the blocks and guide structure. We will report on measurements we have developed using soft X-rays to measure the block copolymers in DSA films. We will also show how we have directly incorporated materials simulation into the data fitting process to extra chemical interactions at the nanoscale from the scattering data.

11:25 a.m.  "Soft X-ray Reflectivity for Quantifying the Chemical Distribution in Thin Films"
Daniel Sunday, National Institute of Standards & Technology

Resonant soft X-ray reflectivity (RSoXR) provides a promising approach towards characterizing the functional group distribution in thin films. Most examples of this technique focus on enhancing contrast between two different phases to better characterize the structural parameters of the film (i.e. layer thickness or interface width). The changes in the optical constant with energy are sensitive not just to the presence of the various chemical bonds in the system, but also their concentration. Because of this sensitivity to the functional group concentration RSoXR should be able to characterize the depth profile of functional groups in a system. This will be demonstrated on polyamide membranes prepared using a layer-by-layer process. The relationship between functional group concentration and optical constants will be calibrated via a series of well controlled reference samples. This is a general approach that can be translated to a variety of systems.

11:40 a.m.  "Optimization of Human-Performance Biosensors: Opportunities in RSoXS and NEXAFS to Elucidate Biomolecular Structure/Function Relationships for Future Sensor Design"
Nicholas Bedford, Air Force Research Laboratory

Wearable FET-based biosensors are identified as candidates for real-time monitoring of biomarkers that correlate with stress and cognition during certain tasks. Typically antibodies-biomarker interactions are used to trigger a sensor response, where small changes in biomolecular conformation upon binding induce a change in the FET gate voltage. Issues exist with larger biomolecules however, where eventual denaturing results in a loss of selectivity. As an alternative, our work focuses on smaller molecule peptide and nucleic acid biological recognition elements (BREs) that exhibit high sensitivity/selectivity properties despite their comparatively disordered structure. To further improve sensor properties, understanding the orientations and structures driving interactions between target biomarkers, corresponding BREs, and the inorganic device is critically important. To better understand these interactions, our group has focused on using various microscopy and non-resonant scattering methods to help correlate sensor properties to binding dynamics/orientation. Though the results to date have been encouraging, obtaining molecular-level structure and orientation information is expected to provide the requisite fundamental knowledge needed to rationally optimize BRE functionality for enhanced sensor properties. To this end, our group has begun to turn our focus to resonant soft X-ray characterization techniques. This talk will summarize our non-resonant X-ray characterization work to date and conclude with future ideas regarding resonant soft X-ray experimentation at NSLS-II.
### Description:

The excellent characteristics of NSLS-II invite the application of coherent x-ray illumination to systems representative of fundamental problems in a wide variety of scientific fields, including Materials Science and Condensed Matter Physics. Indeed several NSLS-II beamlines (Coherent Soft X-ray (CSX-1), Coherent Hard X-ray (CHX), Hard X-ray Nanoprobe (HXN) and Submicron Resolution X-ray Spectroscopy (SRX)) exploit the high coherent flux to image structures and characterize associated dynamics, effectively probing collective and nano-scale ordering, density fluctuations and magnetic correlations. For example, even in these early days of NSLS-II’s user operation, coherent imaging methods have been successfully applied to operando energy storage systems and the mapping of magnetic domains. As NSLS-II and its X-ray instrumentation mature, we anticipate that the brightness of the source will allow the routine extension of coherent scattering techniques into the domain of time-resolved and in situ experimentation. In this light, the workshop aims at gathering scientists interested in the field to discuss technical and data processing limitations experienced in their recent work; brainstorm on challenges; propose developments for current and future imaging experiments, especially as time-resolved applications become mainstream; and highlight topical problems in soft and hard condensed matter that can be effectively tackled. Contributed communications and short student presentations are welcome to supplement the invited talks.

### Workshop Schedule

#### 8:45 a.m.  Continental Breakfast (included)

#### 9:00 a.m.  Opening and Welcoming Remarks

#### 9:10 a.m.  “Bragg Coherent X-ray Diffraction for Nanocrystal Structure and Dynamics”
Ian Robinson, Brookhaven National Laboratory

#### 9:50 a.m.  “Synchrotron Based Approaches for Spatial Resolution of Electrode Reactions”
Esther Takeuchi, Stony Brook University / Brookhaven National Laboratory

#### 10:30 a.m.  Morning Break (included)

#### 11:00 a.m.  “Bragg Coherent X-Ray Diffraction Imaging of Strain in Nanoscale Structures”
Paul Fuoss, Argonne National Laboratory

#### 11:30 a.m.  “Bragg Ptychography: when Crystallography Meets Microscopy”
Virginie Chamard, Aix-Marseille University

#### 12:00 p.m.  Lunch (included) and Group Photo (+ ~30 Discussion)

#### 1:30 p.m.  “Imaging Cells and Brains: Fast, Cool, and in Color”
Chris Jacobsen, Argonne National Laboratory
2:00 p.m. “High-Resolution Hard X-ray Ptychography at SPring-8: Recent Progress and Future Prospects”
Yukio Takahashi, Osaka University

2:30 p.m. “MAUI: Modeling, Analysis and Ultrafast Imaging at Argonne National Laboratory”
Ross Harder, Argonne National Laboratory

3:00 p.m. Coffee Break (included)

3:30 p.m. “Nanoscale Multimodal X-ray Imaging at the Hard X-ray Nanoprobe”
Yong Chu, Brookhaven National Laboratory

3:50 p.m. “CSX Path to Soft Coherent Imaging”
Wen Hu, Brookhaven National Laboratory

4:10 p.m. “Future Possibilities for Coherent Imaging Instrumentation at NSLS-II”
Garth Williams, Brookhaven National Laboratory

4:30 p.m. Roundtable, Discussion and Concluding Remarks

5:00 p.m. Workshop Adjourns

9:10 a.m. “Bragg Coherent X-ray Diffraction for Nanocrystal Structure and Dynamics”
Ian Robinson, Brookhaven National Laboratory

The Bragg Coherent Diffraction Imaging (BCDI) method will be described. BCDI’s greatest strength is to reveal 3D phase-contrast images of the interiors of crystals with image resolution in the 30nm range. It achieves this through the projection of lattice displacements onto the diffraction Q-vector, showing up as a phase shift on a very sensitive scale: one lattice constant results in a phase shift of $2\pi$. Using this new channel of information about the detailed structures of crystals, we have found striking patterns of phase nano-domains within otherwise solid-looking crystals of micron dimension. Since almost all materials are made up of microcrystals, this method has wide application in materials science and engineering and lies at the heart of a case for a new beamline at NSLS-II.

The talk will discuss various materials studied by BCDI: domains introduced in Au by interdiffusion of Cu, faulted misfit domains on the surface of Au induced by Fe diffusion, SAPO-34 zeolite catalyst crystals and the Perovskite $La_{0.5}Ca_{0.5}MnO_3$ (LCMO). I will explain why domain structures are particularly difficult to image using the current methods. Lastly, I will describe some of the challenges and opportunities of time-resolved imaging of the dynamics of internal crystal motions using Free-electron Laser techniques.

9:50 a.m. “Synchrotron Based Approaches for Spatial Resolution of Electrode Reactions”
Esther S. Takeuchi$^{a,b,c}$, Amy C. Marschilok$^{a,b}$, Kenneth J. Takeuchi$^{a,b}$

$^a$Department of Materials Science and Engineering; $^b$Department of Chemistry, Stony Brook University (SUNY), Stony Brook, NY 11794
$^c$Brookhaven National Laboratory, Upton, NY 11973

Full interpretation of electrochemical energy storage mechanisms demands determination of the reaction products as well as identification of their location and distribution. Several approaches have been used to determine the bulk reaction products as well as the spatial location of their formation. Energy dispersive x-ray diffraction (EDXRD) provides a method to achieve spatial resolution of an electrochemical process inside a functioning electrochemical cell, providing the opportunity for tomographic-like data analysis. The approach enables a direct probe of electrode reactions in cells fully encased in their steel housings. The homogeneity of the reaction product formation, the interface where the reaction initiates and the reaction progress as a function of discharge or charge can be effectively mapped. Spectroscopic methods can also be effective for mapping electrochemical reactions at the electrode level and are not dependent on crystalline long range
order. We have effectively used micro-x-ray fluorescence to map electrode surfaces as a function of state of charge to determine both reaction progress and identify parasitic reactions that have occurred within the cell. Further, electrode mapping using transmission x-ray microscopy (TXM) has provided resolution of the discharge reaction and locational information. Further, x-ray absorption near edge structure (XANES) spectroscopic microscopy has been used to identify reaction product formation with further spatial resolution. Micro-extended x-ray absorption fine structure (EXAFS) provides related structural information on the reaction products. Examples of the use of these techniques to elucidate reaction progress and the factors limiting the reactions will be provided.

11:00 a.m.  
**“Bragg Coherent X-Ray Diffraction Imaging of Strain in Nanoscale Structures”**  
Paul Fuoss, Argonne National Laboratory

The physical properties and performance of advanced materials depend strongly on localized structures, and strain within and near those localized structures. I will describe our studies focused on the development and use of coherent diffraction imaging techniques that can map, with exceptional sensitivity and resolution, strain fields around both isolated objects and within continuous films. Using Bragg coherent diffraction imaging, we can measure, with nanometer spatial resolution and picometer-scale sensitivity to lattice distortions, the heterogeneous strain in thin films and correlate these strains with growth behavior. My talk will focus on our recent developments [1-3] of new coherent diffraction techniques that help enable the imaging of both the nanoscale morphological and lattice responses of materials in changing environments, and yield insight into kinetic processes ranging from defect dynamics to phase evolution and growth.


11:30 a.m.  
**“Bragg Ptychography: when Crystallography Meets Microscopy”**  
Virginie Chamard, Aix-Marseille University

Imaging complex crystalline materials at the nanoscale is a major challenge of nanoscience, which calls for a microscopy method combining sensitivity to the crystalline properties, 3D imaging capability, in situ compatibility and high spatial resolution. In this context, the recent advents of x-ray lensless imaging methods, based on Bragg coherent diffraction, have opened promising perspectives [1] filling the gap between direct microscopies (AFM, SEM, TEM) and reciprocal-space based x-ray Bragg diffraction analysis.

3D Bragg ptychography microscopy [2] is a coherent diffraction imaging method developed at third generation synchrotron sources, and which merges concepts developed in inverse microscopy and crystallography. This modality is based on the acquisition of far-field Bragg coherent intensity patterns; It exploits the partially redundant information obtained by scanning a finite beam spot size transversally to the sample, while measuring the corresponding 3D far-field intensity diffraction pattern by scanning angularly the sample along the rocking curve. Instead of lenses, numerical tools are employed to retrieve the lost phase [3] and hence the complex-valued sample scattering contrast. Thereby, it ensures access to truly quantitative information, such as the crystalline displacement field, from which the 3D strain component and crystalline plane rotations can be derived, with nanoscale spatial resolution. 3D imaging of extended crystalline samples is then possible [2, 4], opening Bragg coherent diffraction microscopy to a large range of applications.

In this presentation, the general concepts of Bragg ptychography will be detailed, illustrated by recently proposed developments [5-7]. Finally, we will show how Bragg ptychography can be exploited to bring new insights on the hierarchical crystalline structure of biominerals and promotes thereby the understanding of the mechanisms underlying biomineralization [8].
This project has received funding from the European Research Council (ERC) under the European Union’s Horizon H2020 research and innovation program grant agreement No 695093.

References


2:00 p.m. “High-Resolution Hard X-ray Ptychography at SPring-8: Recent Progress and Future Prospects”
Yukio Takahashi, Osaka University

X-ray ptychography is a method of coherent X-ray diffractive imaging that applies translational diversity, in which the object of interest is scanned in small steps by an overlapping probe, providing redundancy in collected data. So far, X-ray ptychography has been applied to structural imaging of various specimens in biology and materials science at the nanoscale. X-ray ptychography can also provide us with chemical information of a sample by using an X-ray absorption edge. Recently, the X-ray absorption fine structure of nanomaterials has been reconstructed by soft X-ray spectro-ptychography[1]. Extending this approach to the hard X-ray region will enable us to visualize the chemical state of nanostructures buried within thick samples. However, a limitation of this method is the weak absorption of incident X-rays in the hard X-ray region. To improve the convergence of the phase retrieval for complex-valued images in X-ray spectro-ptychography, we propose the addition of a constraint based on the Kramers-Kronig relation to phase retrieval algorithms[2]. We applied it to the visualization of the spatial distribution of Ce$^{3+}$ and Ce$^{4+}$ in each particle of Ce$_2$Zr$_2$O$_x$ in a three-way conversion catalyst system[3]. The dynamic range of X-ray detectors is a key factor limiting the performance of X-ray spectro-ptychography. Dark-field X-ray ptychography[4,5], which compresses the dynamic range of intensities of diffraction patterns, will become a promising approach to solve the problem.

References


2:30 p.m. “MAUI: Modeling, Analysis and Ultrafast Imaging at Argonne National Laboratory”
Ross Harder¹, Mathew Cherukara¹, Kiran Sasikumar¹, Tom Peterka¹, Ian McNulty¹, Nicola Ferrier¹, Todd Munson¹, Sven Leyffer¹, Subramanian Sankaranarayanan¹ and Haidan Wen¹
¹Argonne National Laboratory, USA
rharder@aps.anl.gov

Coherent x-ray diffractive imaging (CXDI) can now reach down to sub ten nanometer structural imaging of materials[1]. When done in the Bragg geometry one can also image distortions of the lattice with 10−5 sensitivity [2, 3]. Bragg CDI is also highly compatible with in-situ and operando studies of materials owing to the relatively large free space around the sample. Recently we have conducted imaging experiments with both catalytic systems and ultrafast laser pump – x-ray probe of energy transport by phonons in nanomaterials[4,5]. To quantify the response seen in the materials there is an increased requirement for image analysis to understand the physical processes occurring.

Advanced image analysis and molecular dynamics (MD) simulations are now scaling in the opposite direction of CXDI. These computational methods are reaching UP to the length/time scales achieved in the
imaging experiments. Image meshing techniques can be used to create models of the actual samples in an experiment, which can then feed into multi-million atom MD and finite element simulations over hundreds of picoseconds[5].

Building a complete workflow to understand nanoscale phenomena with atomistic origins is the goal of the MAUI (Modeling, Analysis and Ultrafast Imaging) project at Argonne National Laboratory. Specialists in coherent imaging, ultrafast laser science, 4D image analysis, math, and computer science have teamed up with molecular dynamics simulations experts to develop these tools.

This talk will focus on recent efforts and results coming out of the MAUI team.

References

3:30 p.m. “Nanoscale Multimodal X-ray Imaging at the Hard X-ray Nanoprobe”
Yong. S. Chu, Hanfei Yan, Xiaojing Huang, Mingyuan Ge, Hande Ozturk, Evgeny Nazaretski, and Petr Ilinski
NSLS-II, Brookhaven National Laboratory

The Hard X-ray Nanoprobe (HXN) at NSLS-II delivers a world-leading imaging resolution for user science experiments. Significant efforts have been made to offer a suite of imaging techniques, so that different properties of the sample can be analyzed simultaneously. The techniques include fluorescence, transmission, phase-contrast imaging, diffraction, spectroscopy, and ptychography (both transmission and Bragg). Presentation will describe the current and near-future imaging capabilities.

3:50 p.m. “CSX Path to Soft Coherent Imaging”
Wen Hu, Andi Barbour, Claudio Mazzoli, and Stuart Wilkins
NSLS-II, Brookhaven National Laboratory

The Coherent Soft X-ray Scattering beamline (CSX-1) is a canted undulator beamline at sector 23-ID providing coherent soft x-ray scattering and imaging with world-leading high-coherent flux and detectors. Endstation instrumentation allows experiments using X-ray Photon Correlation Spectroscopy, Scanning Diffraction Microscopy, Resonant X-ray Scattering, Surface X-ray Diffraction, Fluorescence and Coherent Diffraction Imaging. CSX-1 is dedicated to host a variety of Coherent Soft X-ray Imaging and Scattering techniques, where sample is typically imaged without x-ray "lenses", for investigating scientific issues in soft condensed matter under various sample environments (temperature, magnetic or electric fields). In this presentation, we will describe the capability and on-going development at CSX-1 toward Coherent Soft X-ray Imaging, and aim to have discussion on the soft coherent imaging opportunities and the needs of the community.
Workshop 8
New Detectors for New Light Sources
May 17, 2017

Location: Bldg. 488, Berkner Hall, Conference Room B

Organizers: Daniel Allan, NSLS-II-BNL (dallan@bnl.gov)

Description: This workshop is an interactive tutorial on how NSLS-II’s data acquisition software can be used to perform an experiment and enable sophisticated improvisation at the beamline. NSLS-II has developed open-source software for integrated data acquisition, management, and analysis. The software consists of a number of cooperative libraries (‘ophyd’, ‘bluesky’, ‘databroker’ and others). The user-facing control interface, ‘bluesky’, is independent of the underlying control system: it enables beamline staff and users to develop sophisticated experiment procedures without any special knowledge of EPICS. Workshop attendees will be guided through a “cookbook” of practical examples, and they will try them on a simulated beamline via their Internet browser. Cookbook recipes will include automatically recovering from a beam dump in the middle of the night; incorporating adaptive logic into an experiment procedure; creating custom live visualization and data processing pipelines; and exporting data to take home in any format. Prior Python experience will not be necessary to follow the tutorial, but some general programming experience will assumed.

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<tr>
<td>12:00 p.m.</td>
<td>Lunch (included)</td>
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<td>1:00 p.m.</td>
<td>Interactive Software Tutorial</td>
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<td>Daniel Allan, Brookhaven National Laboratory</td>
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<td>3:00 p.m.</td>
<td>Coffee Break (included) and Group Photo</td>
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<td>Workshop Concludes</td>
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Workshop 9
Probing Dynamics in Soft and Hard Condensed Matter with Coherent X-rays
May 17, 2017

Location: Bldg. 735, Center for Functional Nanomaterials (CFN), Large Conference Room

Organizers: Oleg Gang, CFN-BNL and Columbia University (ogang@bnl.gov)
Jeffrey Kysar, Columbia University (jk2079@columbia.edu)
Masa Fukuto, NSLS-II-BNL (fukuto@bnl.gov)

Description: The mechanical properties of nanostructured materials can significantly deviate from their conventional bulk counterparts due to the contribution of surface effects, grains and the effect of nanoscale architecture. Potentially, such materials can exhibit the highly targeted performances: being strong yet light, be hard but not brittle, and respond to stress and temperature in the desired way. Moreover, they can give access to unique properties of mechanical metamaterials.

Creating these 3D materials in a designed manner is challenging problem. Conventional fabrication methods are not well positioned for fabricating of 3D structures with the desired mechanical response. On other side, chemical synthesis and self-assembly methods offer a limited control over the architecture of materials. This in contrast to biological systems, which often demonstrate a remarkable level of control. Thus, the new approaches are needed for fabrication of material with tailored mechanical properties.

Experimental characterization of nanoscale and nanostructured materials is quite challenging due to the need to measure nm-scale displacements and nN-scale forces. Nanoindentation and MEMS actuators provide the most versatile experimental platform for this purpose. Performing the experiments in-operando a scanning electron microscope provides the opportunity to observe failure mechanisms and to measure heterogeneous deformation fields. Comprehensive insight on multiscale response of the materials under stress can be probed by x-ray scattering methods.

The workshop will bring together scientists in the area of material fabrication, nano-mechanical testing and multiscale in-situ characterization to discuss the advances and needs for advancing fabrication of nanomaterials with tailored mechanical response and revealing their structure-function relationship using in-situ methods.

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<td>8:30 a.m.</td>
<td>Continental Breakfast (included)</td>
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<td>8:30 a.m.</td>
<td><strong>Introduction and Welcome</strong></td>
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<td>Oleg Gang, Brookhaven National Laboratory</td>
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<td>8:35 a.m.</td>
<td><strong>“Multiscale Experiments to Inform and Validate Multiscale Models”</strong></td>
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<td>Jeff Kysar, Columbia University</td>
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<td>9:00 a.m.</td>
<td><strong>“Combinatorial Micromechanics”</strong></td>
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<td>Jeffrey Wheeler, ETH Zurich</td>
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<td>9:30 a.m.</td>
<td><strong>“A New Type of Superelastic and Shape Memory Materials: ThCr2Si2-Structured Novel Intermetallic Compounds at Small Length Scales”</strong></td>
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<td>Seok-Woo Lee, University of Connecticut</td>
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<td>10:00 a.m.</td>
<td>Morning Break (included) and Group Photo</td>
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Micromechanical testing has made significant progress in the last few decades. Advances in instrumentation and techniques have developed new geometries for measuring uniaxial strength and fracture toughness at very small length scales [1]. In addition to increasing the test space envelope in terms of smaller sizes, the development of displacement controlled systems has allowed these properties to be investigated over a wide range of strain rates, even within single samples using strain rate jump and stress relaxation techniques [2]. Using new, high speed actuators, the available test space has also been expanded to reach the high strain rate regime (>103 s⁻¹). To complete the testing envelope, significant effort has been spent on achieving high temperature testing [3], and recently cryogenic temperature testing has also been achieved [4]. By combining all these capabilities, the micromechanical testing envelope has grown to encompass a significant range of testing temperatures (-100 to 600 °C) and over eight orders of magnitude in strain rates (10⁻⁵ to 10³ s⁻¹). This creates the opportunity for plastic deformation mechanism mapping of materials at small scales over a wide range of homologous temperatures.

Diffusion couples have long been a fundamental technique in materials science, allowing the exploration of phase diagrams and diffusion constants. With the advent of the Materials Genome Initiative, diffusion couples and multiples are now being used as a high throughput means to investigate a wide range of materials properties [5]. However, so far only the most fundamental micromechanical technique (nanoindentation) has been used to interrogate mechanical properties of diffusion couples. Here, the potential of applying advanced micromechanical techniques to diffusion couples will be demonstrated in the case of the Al-Cu binary system.
“A New Type of Superelastic and Shape Memory Materials: ThCr2Si2-Structured Novel Intermetallic Compounds at Small Length Scales”
Seok-Woo Lee, University of Connecticut

Crystalline, superelastic materials typically exhibit large recoverable strains due to the ability of the material to undergo a reversible phase transition between martensite and austenite phases. Applicable to various alloys, ceramics and intermetallic compounds, this reversible transition serves as a general mechanism for superelasticity and shape memory effect. Recently, we noticed that ThCr2Si2-structured intermetallic compounds exhibit a reversible phase transition between a tetragonal (or orthorhombic) phase to a collapsed tetragonal phase under compression along c-axis of the unit cell by making and breaking Si-Si type bonds. This process has nothing to do with martensitic transformation. This unique reversible phase transformation process motivated us to investigate their potential as a superelastic and shape memory material.

In this study, we studied CaFe2As2, which is one of ThCr2Si2-structured intermetallic compounds and has been extensively studied in the field of solid-state physics due to its remarkable pressure sensitive electronic, magnetic and superconducting properties. Millimeter-sized single crystals were grown by Sn-flux solution growth technique, and micropillar compression was performed along c-axis to characterize their mechanical behavior. We confirmed CaFe2As2 exhibits over 3 GPa strength and over 13% recoverable strain, both of which lead to the ultrahigh elastic energy storage and release 10~1000 times higher than that of conventional high strength materials. Furthermore, we found the exceptional repeatability of cyclic deformation and superior fatigue resistance, compared to shape memory ceramics, which is known as the current state-of-the-art shape memory material. Furthermore, our in-situ cryogenic neutron scattering experiment under pressure showed that CaFe2As2 exhibits linear shape memory effect below 100 K by restoring the original orthorhombic phase from the collapsed-tetragonal phase. This ultra-low temperature shape memory effect could be used to develop a cryogenic linear actuation and sensor technology for deep space exploration. Note that our observation is only one manifestation of a wider class of such transitions found in significant number of ThCr2Si2-structured intermetallic compounds Thus, we believe that our results will represent a paradigm shift in the area of superelastic and shape memory materials with a new phase transformation mechanism, enable an innovative design of cryogenic linear actuators, sensors, and switching devices in extremely cold environments, and more broadly, suggest a mechanistic path to a whole new class of shape memory materials.

“Recent Advances in Materials Characterization Using Instrumented Indentation Tests”
Warren Oliver, Nanomechanic Inc.

Three new instrumented indentation testing techniques will be discussed. They include high temperature, high strain rate and two dimensional testing.

Instrumented indentation testing provides unique opportunities to study strain rate effects on the strength materials. In situ high temperature indentation testing to measure the relationships between temperature, strain rate and strength has received considerable interest in recent times. In this regard, data from in situ dynamic nanoindentation testing up to 550 C on commercial purity aluminum will be presented and compared to the values from literature. The same concepts can be applied to measure properties at high strain rates. High strain rate indentation testing results will be presented and compared to macroscopic literature results.

Finally, the first results from a new system which retains the high performance measurement capabilities in the direction normal to the surface of the sample and adds the equivalent signals parallel to the surface will be presented. The same sensitivity, range and dynamic performance (including frequency specific experiments) are available simultaneously and continuously in both directions. The ability to measure not only load and displacement but stiffness and phase angle at specific frequencies parallel to the surface continuously and simultaneously with these same measurement in the normal direction has resulted in entirely new results concerning the onset of sliding between two bodies in contact. Unique new data concerning the initiation of slip at micro asperities, friction and wear, lubrication, scanning surface topology, mechanical property mapping and multidimensional characterization of structures can now be investigated.
“From Experimentation to Understanding in Engineering Devices: In Operando Testing”
Douglas Stauffer, Bruker Nano Surfaces

Materials behavior is often dominated by highly localized phenomena, and the ability to probe these local properties for engineering devices is critical. Often these devices are operating in environments with large differences in temperature and pressure: from the high vacuum and cold of space to the high temperature and high pressure inside a deep-water oil well. Here, a synopsis of three different materials systems in the environments of interest is presented.

Fatigue crack growth has long been investigated via post mortem analysis, leading to a phenomenological understanding of crack initiation at stress concentrators. However, post-mortem investigations can be very difficult for ultrathin grained materials, such as the Cu thin film in this study, and give little insight as to the dynamic changes in the material under cycling. In situ TEM studies can give a wealth of information, such as grain size, grain orientation, continuous monitoring of crack length/direction/radius, and plasticity present at the crack tip. Here, in situ fatigue is demonstrated using cyclic mechanical loading experiments at frequencies up to several hundred Hz. More than $10^6$ cycles can be reached within one hour. Moreover, the nanometer-scale spatial resolution of the TEM allows the observation of “incipient” crack growth rates of $<10^{-12}$ m$\cdot$cycle$^{-1}$ very near to the minimum threshold stress intensity factor. With Daniel C. Bufford, William M. Mook, S.A. Syed Asif, Brad L Boyce, and Khalid Hattar.

Steel is an incredibly important structural material, providing a literal framework for modern society. While the ductile to brittle temperature transition is well known, and for the most part well understood, localized measurements of this phenomena in this complex material are less common. Here, a simple low-carbon steel, 1018, is tested from -120 to 25°C to examine the contribution of the ductile to brittle temperature transition of each of the two critical phases: ferrite and pearlite towards catastrophic failure. With Anqi Qiu

Diffusion aluminide bond coats are compositionally and microstructurally graded materials with significant variation of engineered mechanical properties across the cross-section. The thermal cycles treatments of bond coats during service leads to extensive interdiffusion of elements between the substrate and the coating which create further gradient in chemistry and microstructure and hence modifies properties. In situ micropillar compression testing up to 800˚C helps to elucidate the mechanical behavior of individual bond coat layers. With Sanjit Bhowmick, Eric Hintsala, and S.A. Syed Asif.

“In-Situ Mechanical Testing and Fracture Processes in Polymer-Grafted Nanoparticle Assemblies”
Lawrence Drummy, Air Force Research Laboratory

Three dimensional assemblies of polymer-grafted “hairy” nanoparticles (HNPs) are of current interest for a wide array of mechanical and electrical applications. The areal grafting density of the polymer chains on the nanoparticle surfaces, and the molecular weight of the grafted polymers, determine the resulting interparticle spacing and volume fraction of the polymer and nanoparticle constituents. Because the polymer is chemically grafted to the particle surface particle-particle contacts are eliminated, as opposed to a physical blending process in which nanoparticle agglomeration is typically observed. The mechanical properties of HNPs films are therefore dominated by the polymer-polymer entanglements and the ordering in the nanoparticle assembly. Previous studies of HNP thin films have largely relied on nanoindentation, due to the challenges of preparing sub-micron testing specimens. The emergence of microelectromechanical systems (MEMS) techniques for fabricating devices and microscale specimen preparation using focus ion beam (FIB) allows for in situ study of failure process of HNP assemblies. Previous results in ex-situ tests have shown that crack processes dominate deformation in HNP assemblies with low grafting density, but crazing occurs for assemblies with high grafting density. As with linear polystyrene, molecular weight and strain rate also impact the transition from crack to craze. These correlations between HNP architecture and subsequent failure mode refines the HNP design space for the synthesis and fabrication of assemblies with defined mechanical properties. In this study fundamental processes of craze initiation, the effect of film thickness, and the role of silica nanoparticles are examined in polystyrene-silica HNP assemblies synthesized using the grafting-from method.
Energy dissipation mechanisms are critical to the development of tough hydrogels with the double network being the most well established route. One challenge with the double network design is the toughness is derived from the breaking of covalent bonds in the sacrificial 2nd network. One alternative to the rupture of covalent bonds is the use of non-covalent interactions, such as ionic bonds, hydrogen bonds or hydrophobic aggregates, to act as the sacrificial network. In this case, the bonds can be reversible, so the energy dissipation should also be reversible. However, the exact mechanisms associated with the breaking and reforming of these non-covalent bonds are not clear. In this talk, I will discuss the use of a model hydrogel material that is based on a random amphiphilic copolymer. The hydrophobe is perfluorinated and this leads to aggregation of the fluorinated moieties into well-defined nanoscale aggregates. The higher electron density of the fluorinated domains provides x-ray contrast to enable the characterization of the nanostructure. As the crosslinks are dynamic and only based on hydrophobic association, the evolution of the nanostructure as the hydrogel is uniaxially stretched is strongly dependent on the stretching rate. Changing the stretching rate by 3 orders of magnitude leads to significant differences in the nanoscale anisotropy developed in the sample during deformation. This difference in the change in the nanostructure can be directly related to the mechanical response of the hydrogel (stress-strain curve). If time permits, a brief description of the structural recovery on cessation of deformation will be provided to provide insight into the reversibility of these tough hydrogels and the relevant time scales.

Although the word “hierarchy” originally meant “rule of a high priest,” nothing seems further from ecclesiocratic dictate than the familiar microscale hierarchy we find in nature: the organic, twisting form of a biomaterial. Yet, hierarchy, with one level built upon another, is observed in all biosystems and is required for a functional synthetic assembly. A mineral-organic hybrid can be viewed as a two-level hierarchy, operating on two length scales to strengthen the system against cracks and flaws. In this talk I will review two-level and multi-level hierarchical materials with enhanced mechanical properties. Most of these systems incorporate comparatively harder and softer sub-components, the latter of which may be crystalline. This enables x-ray scattering to effectively map the composition across many length scales, and simultaneously, probe the system’s response to mechanical stimulation. The discussion will reinforce an important issue: one of our main challenges now is the hierarchy of data and metadata that must be managed to make the most of our experiments.

Nature produces a remarkable diversity of intricately architectured mineralized composites that in many instances far exceeds the performance of their modern engineering analogs. Despite significant investigations into structure function relationships in these complex biological materials, in many instances, there is a lack of critical information regarding the specific functional roles of many components of these structural hierarchies. Here we introduce the technique of multi-material additive manufacturing, which we employ as a research tool to unravel the functional complexities of a wide range of biological materials including laminated composites, photonic architectures, and low drag surface coatings.
3:00 p.m.  “Probing Nano-mechanics of Materials by X-ray Imaging”
Karen Chen-Wiegart, Stony Brook University/Brookhaven National Laboratory

X-ray imaging techniques, including tomography, characterize the morphology of materials. When conducted in situ or operando, x-ray imaging can be particularly powerful in revealing processing-structure-property relationships. This talk aims to provide a brief overview about utilizing x-ray imaging, including tomography, to probe nano-mechanical properties of materials. Descriptions on beamline capabilities of NSNL-II will also be introduced. Examples include full-field x-ray nano-tomography for the study of micro-structural evolution and degradation of materials under stress; systems such as metal alloys, porous metals and energy storage materials will be addressed. In addition, the structure information obtained by x-ray imaging can be used in computational simulations (e.g. finite element analysis) to investigate mechanical properties. Novel imaging techniques such as Bragg coherent diffraction imaging, which provides strain sensitivity when imaging nano-structure, will also be discussed.

3:30 p.m.  “Sub-Å-resolution Elasticity and Friction in 2D Van der Waals Materials”
Elisa Riedo, City University of New York ASRC

Two-dimensional (2D) materials, such as graphene and MoS2, are a few-atomic-layer thick films with strong in-plane bonds and weak interactions between the layers. The in-plane elasticity has been widely studied in bending experiments where a suspended film is deformed substantially; however, little is known about the films’ elastic modulus perpendicular to the planes, as the measurement of the out-of-plane elasticity of supported 2D films requires indentation depths smaller than the films’ interlayer distance.

Here, we present a new method to perform sub-Å-resolution indentations to measure the perpendicular-to-the-plane elasticity in 2D materials and nanotubes [1], and its implications for graphene and graphene oxide films. This method, called Å-indentation goes beyond the standard nanoindentation approach and allows for high resolution elasticity measurements of films that are atomically thin and extremely stiff.

Our indentation data, combined with semi-analytical models and density functional theory are then used to study the perpendicular elasticity of a few-layers thick graphene and graphene oxide films. We find that the perpendicular Young’s modulus of graphene oxide films reaches a maximum when one complete water layer is intercalated between the graphitic planes. This non-destructive methodology can map interlayer coupling and intercalation in 2D films.

Furthermore, we will discuss our recent work on the interplay between number of layers, structure, defects and friction in MoS$_2$ films.

BNL MAP
Berkner Hall Exhibitor Layout

Exhibitors & Sponsors
Chemistry Department
Hamilton Seminar Room
Building 555

**Monday, May 15**
Table #60 – greateyes GmbH

**Wednesday, May 17**
Table #64 - greateyes GmbH
Table #65 - Huber Diffraction USA

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CFN Department
Large Conference Room
Building 735

**Monday, May 15**
Table #56 – VAT, Inc.
Table #57 – Scientific Instruments

**Wednesday, May 17**
Table #59 – VAT, Inc.
Table #58 - Scientific Instruments
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Exhibitor Presentations

In a special offering, several exhibitors will also be demonstrating their products on Tuesday, May 16 at mini-workshops in Berkner Hall in Conference Rm. C. Please review the following schedule. We hope you can attend!

<table>
<thead>
<tr>
<th>Time</th>
<th>Exhibitor</th>
<th>Presentation Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:30 a.m.</td>
<td>greateyes, GmbH</td>
<td>Scientific CCD Cameras for EUV and X-Ray Applications</td>
</tr>
<tr>
<td>2:00 p.m.</td>
<td>Hitachi High-Technologies Science America</td>
<td>Advanced Silicon Drift Detectors for Synchrotron Applications</td>
</tr>
</tbody>
</table>

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SPECS manufactures systems and components for surface analysis, based on electron spectroscopy and imaging techniques such as SPM and LEEM. In customized systems SPECS integrates facilities for thin film preparation and in-situ analysis in Vacuum systems from UHV to high pressures.

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508-618-1292
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From our earliest days in the power conversion industry, through today, Spellman has always played a major role in supporting basic and applied scientific research. Collaborating with leading researchers in fields as diverse as physics, chemistry, medicine, biology, electronics, materials, and astronomy, we have developed products that enabled exciting advances in many disciplines. And, in many cases, were subsequently adopted into mainstream industries and applications around the World.

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sales@tru-stone.com

Starrett Tru-Stone Technologies specializes in precision granite machine bases & assemblies. We partner with you to add expertise in design collaboration, high-quality on-time manufacturing and complex assembly for your precision base. In addition to granite bases, Tru-Stone techs install precision rails, air mounts, brackets, pneumatic systems and cabling. Custom stands are also provided. Materials beyond granite include ceramic, carbon fiber materials.

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**Toyama Co. Ltd.**

3816-1 Kishi
Yamakita-machi
Ashigarakami-gun, Kanagawa 252-0003 JPN
+81-46-579-1411
sales@toyama-jp.com

Toyama is a Japanese supplier of ultra-precision systems for experimentation at the cutting edge of science. In April 2015 Toyama opened its new state-of-the-art facilities some 70 kilometres southwest of Tokyo. Here, Toyama’s 150 full-time staff are working together with scientists and engineers from leading research institutes worldwide to develop instrumentation in fields as diverse as synchrotron radiation, nuclear physics, semiconductor technology, and fusion research.

Toyama is proud of its traditions of excellence in engineering design, manufacturing, commissioning, and service support. Toyama’s instrumentation is held in high regard by many engineers and scientists. Our purpose is to continue to support research and development activities at the cutting-edge of science. It is our intention to be the “Best Partner for Scientists”.

**VACOM Vakuum Komponenten & Messtechnik GmbH**

In den Brückenäckern 3
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+49 3641 4275-25
info@vacom.de

VACOM ranks among the European market leaders for vacuum technology. Its leading brand Precision & Purity stands for the highest demands in UHV, XHV, and UCV. Core areas of expertise are vacuum hardware, electrical feedthroughs, vacuum measurement, vacuum optics, and ion getter pumps. VACOM is partner in high-tech industries and research institutes e.g. in the field of analytics, semiconductors, optics, and accelerator technologies worldwide.

**Vacuum Solutions Group**

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Teaneck, NJ 07666
201-692-7924
sales@vacuumsolutions.com

Vacuum Solutions Group represents MPF, ColdEdge, Osaka Vacuum, Mewasa, HVA valves, AVT, Anderson Dahlen, and Brooks.
VAT, Inc. will be located in Bldg. 735, Center for Functional Nanomaterials (CFN), Large Conference Room on Monday, May 15 at the “Spectro-microscopy at the Nanoscale: Exploring Chemical, Electronic and Magnetic Properties of Novel Materials” Workshop.

VAT, Inc. will be located in Bldg. 735, Center for Functional Nanomaterials (CFN), Large Conference Room on Wednesday, May 17 at the “Nano-mechanics: From Material Fabrication to In-Operando Characterization” Workshop.

VAT is the global technology leader and supplier of high-end vacuum valves. VAT vacuum valves are mission-critical components in the semiconductor industry, in research and science as well as in advanced manufacturing processes of innovative products such as portable devices, flat screen displays or solar panels. We develop our products in close cooperation with the leading equipment suppliers worldwide. With manufacturing sites in Haag (Switzerland) and Penang (Malaysia), subsidiaries in the USA, Asia and Europe we are where our clients are. Fifty years of experience in the vacuum industry and over 1,400 highly-qualified employees guarantee that clients benefit from outstanding products and related value-added service.

W-IE-NE-R Plein & Baus Corp. is providing a full line of electronics for detector read-out, data acquisition, experiment control and diagnostics.
- WIENER: low voltage power supplies and systems, powered chassis [www.wiener-d.com]
- ISEG: High voltage power supplies, modules and multi-channel systems [www.iseg-hv.com]
- MESYTEC: analog read-out electronics, amplifier, discriminators, VME ADC/QDC/ digitizers [www.mesytec.com]
- GBS: Multi-channel analyzers [www.gbs-elektronik.de]

XIA LLC develops and sells advanced digital signal processors for use with X-ray and gamma-ray detectors and related instruments with applications at synchrotrons and other research facilities. We specialize in high-rate multi-channel spectroscopy systems. XIA is based in Hayward, California, USA, and our multi-lingual staff and overseas representatives support product sales in over 30 countries on six continents.
Accommodations

Accommodations on the BNL Site

Reservations: Housing is very limited. Space is assigned on a first-come, first-served basis. For rates and availability, please contact the Housing Office at (631) 344-2541 or housing@bnl.gov.

Housing charges must be paid to the Housing Receptionist on arrival.

Check-Out time is 3:00 p.m. Before leaving, return your keys to the Housing Office.

The Housing Office is open Monday through Friday, 8:00 a.m. to 10 p.m., and also on Sunday from 4 p.m. to 10 p.m. Those arriving or leaving at other times may pick up or drop off keys at Police Headquarters, Building 50.

Accommodations Offsite (*Roundtrip shuttle service will be provided to BNL from the hotels)

East Wind Long Island
Special Users’ Meeting / BNL Rate - $126.00 - includes a breakfast voucher to Myra’s Cafe, free high speed wireless internet, indoor swimming pool and 24 hour gym. Free shuttle service to and from BNL. Upon check-in, please be sure to inform the front desk that you will be requiring the shuttle service to/from BNL.

5720 Route 25A
Wading River, NY 11792
(631) 846-2337
Exit 68 off the LIE
Est. Travel Time: 19 minutes 10.5 Miles from BNL
Estimated Travel Time from Long Island MacArthur Airport to East Wind: 36 mins / 27.1 miles.

The special room rate will be available until April 30, 2017.

Fairfield Inn - Marriott
Special Users’ Meeting / BNL Rate - $130.00 - includes free continental breakfast, including Hot Breakfast Sandwiches and Hot Breakfast Quiche, free high speed wireless internet, indoor swimming pool and Jacuzzi, fitness center, free shuttle service to LI Islip Airport and Ronkonkoma Train Station and morning and afternoon shuttle service to and from BNL. Upon check-in, please be sure to inform the front desk if you require shuttle service to/from BNL.

2695 Route 112
Medford, NY 11763
(631) 447-6200
Exit 64 off Long Island Expressway (LIE)
Est. Travel Time: 18 minutes 9.1 Miles from BNL
Estimated Travel Time from Long Island MacArthur Airport to SpringHill Suites: 16 mins / 10.32 miles.

The special room rate will be available until May 1, 2017.

SpringHill Suites by Marriott
Special Users’ Meeting / BNL Rate - $130.00 - King Studio - includes free hot buffet breakfast, free high speed wireless internet, fitness center, indoor pool. Upon check-in, please be sure to inform the front desk that you will be requiring the shuttle service to/from BNL.

2 Sawgrass Drive
Bellport, NY 11713
(631) 924-0090
Exit 68 off the LIE
Estimated Travel Time: 13 mins/7.93 miles from BNL
Estimated Travel Time from Long Island MacArthur Airport to SpringHill Suites: 16 mins / 10.32 miles.

The special room rate will be available until April 25, 2017.

Hyatt Place Long Island East End
Special Users’ Meeting / BNL Rate - $130.00 - includes free continental breakfast, free high speed wireless internet, fitness center. Upon check-in, please be sure to inform the front desk that you will be requiring the shuttle service to/from BNL.

451 E. Main Street
Riverhead, NY 11901
631-208-0002
Estimated travel Time: 15 minutes 10.5 Miles from BNL

The special room rate will be available until April 14, 2017.
Offsite Transportation

Trains

The Long Island Railroad serves all of Long Island with service to New York City’s Penn Station; connections are available from there to Amtrak and regional lines.

The closest Long Island Railroad Station to BNL is in Mastic/Shirley; however, trains arrive and depart more frequently at Patchogue and Ronkonkoma. To find schedules and more information, call (516) 822-5477, or visit the World Wide Web site: http://www.mta.nyc.ny.us/lirr/index.html

To get to the Mastic/Shirley LIRR station, take William Floyd (Rte. 46) south of the Lab, past the LIE, Route 27 and Montauk Highway. The parking lot is on the left just after the railroad tracks.

To get to the LIRR Ronkonkoma station, take the LIE to Exit 60, go south, and follow the signs. Parking here is sometimes scarce on weekdays, but the trains run early every hour and the trip takes only an hour and a half. Or, take the Lab car service.

The Port Jefferson station has fewer trains that take more time than Ronkonkoma trains, but the station is closer to the Lab than Ronkonkoma. Take Rte. 46 north to its end at Rte. 25A, following it for 15 miles and taking the right fork toward Port Jeff. At the T intersection, take a right; the station is on the south side of the tracks on the right side of the road. Passengers from Port Jeff need to change trains once (get off, stand at the same platform, get on the next train) to get to Manhattan.

Laboratory Cars/Train Shuttle

The BNL Transportation Office, Bldg.400A, ext. 2535, provides transportation to meet the Long Island Railroad (LIRR) train from New York City arriving in Ronkonkoma at 8:59 a.m., Monday through Friday, and also to catch the LIRR train to New York City leaving Ronkonkoma at 4:46 p.m., Monday through Friday. Due to limited seating, reservations are required for this service. Please telephone ext. 2535, email transportation@bnl.gov or go to Bldg. 400A.

Taxis

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<thead>
<tr>
<th>Taxi</th>
<th>Phone</th>
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<tbody>
<tr>
<td>Colonial Taxi</td>
<td>(631) 589-7878</td>
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<tr>
<td>Courtesy Taxi</td>
<td>(631) 395-5237</td>
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<tr>
<td>Four Ones Taxi Service</td>
<td>(631) 281-8581</td>
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<tr>
<td>Lindy’s Taxi</td>
<td>(631) 654-3456</td>
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<tr>
<td>Sunset Taxi</td>
<td>(631) 588-8844</td>
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<tr>
<td>Village Taxi</td>
<td>(631) 588-1055</td>
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Rental Cars

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<tr>
<th>Rental Car</th>
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<tbody>
<tr>
<td>Alamo</td>
<td>(800) 327-9633</td>
</tr>
<tr>
<td>Avis</td>
<td>(800) 331-1212</td>
</tr>
<tr>
<td>Budget</td>
<td>(800) 527-0700</td>
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<tr>
<td>Dollar</td>
<td>(800) 800-4000</td>
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<tr>
<td>Enterprise</td>
<td>(800) 325-8007 ~ onsite at BNL!</td>
</tr>
<tr>
<td>Hertz</td>
<td>(800) 654-3131</td>
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<tr>
<td>National</td>
<td>(800) 227-7368</td>
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<tr>
<td>Rent-A-Wreck</td>
<td>(800) 535-1391</td>
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<tr>
<td>Thrifty</td>
<td>(800) 367-2277</td>
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Airport Limousine Services

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<tr>
<th>Service</th>
<th>Phone Numbers</th>
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<tbody>
<tr>
<td>Airports Only</td>
<td>(631) 291-6290</td>
</tr>
<tr>
<td>Chris Dee Limousines</td>
<td>(631) 979-3824</td>
</tr>
<tr>
<td>Crestwood Limousine</td>
<td>(631) 399-5196, Cell (516) 457-6124</td>
</tr>
<tr>
<td>Dynamic Limousines</td>
<td>(631) 291-6290</td>
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<tr>
<td>Elegant Limousine</td>
<td>(631) 345-5541</td>
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<tr>
<td>Executive Limo</td>
<td>(631) 696-8000</td>
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<tr>
<td>LI Limo</td>
<td>(631) 234-8400</td>
</tr>
<tr>
<td>Tran-Star Executive</td>
<td>(800) 894-7827</td>
</tr>
<tr>
<td>Winston Transportation</td>
<td>(631) 924-1200</td>
</tr>
</tbody>
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Onsite Transportation

On-Site Shuttle Bus

The On-Site Brookhaven Lab Courtesy Van offers on-call, door-to-door service between the hours of 8:30 a.m. and 4:15 p.m., Monday through Friday, excluding holidays. Please call extension 2714 for pickup. Please be prepared to give the following information: name; telephone extension; location of pickup; location of drop-off; and number of passengers.

Requests are accepted on a first-come, first-served basis. Be prepared to meet the van at the main entrance of your building. In order for us to be able to serve as many customers as possible, please be ready to board the van before making the call for pickup. Pick-ups can be arranged by calling ext. 2714 and providing your name, telephone extension, location of pickup, location of drop-off and number of passengers.

Computers, Phones & Messages

Computer terminals are located in Berkner Hall for use in logging on to your own computer or accessing your email during the meeting.

Messages can be left for you at the Conference Desk. The telephone number (during the meeting only) is (631) 344-3548. Messages will be posted on a bulletin board in Room D (Conference Desk).

A fax machine is located in Berkner Hall for those who require faxing services. The phone number is (631) 344-2069. See the Conference Desk for assistance in using the fax machine.
Nominees for the 2017-19
NSLS-II Users’ Executive Committee

Wilson Chiu
University of Connecticut
Mansfield, CT

Wilson Chiu has been with the University of Connecticut since 1999, where he is currently Professor of Mechanical Engineering. He has been a regular synchrotron user for over 10 years. His research uses x-ray imaging at NSLS/NSLS-II, APS, and SSRL to investigate the role of 3-D transport and electrochemistry in energy materials for fuel cell, gas separation membrane, and nuclear waste form applications. In collaboration with beamline scientists, he developed imaging techniques such as absorption contrast nanotomography, XANES nanotomography, phase contrast imaging, and high temperature in situ imaging with controlled sample gas environment. Wilson Chiu is a fellow of the American Society of Mechanical Engineers and the Connecticut Academy of Science and Engineering. He serves as the Editor-in-Chief for the Journal of Electrochemical Energy Conversion and Storage, and chair of the Full field X-ray Imaging (FXI) Beamline Advisory Team (BAT) at NSLS-II. He also served on the 2015 SSRL Imaging Beam Line Review Committee. Wilson Chiu is interested in advancing the x-ray imaging program and facilitating access for the x-ray imaging user community to NSLS-II.

Riccardo Comin
Massachusetts Institute of Technology
Cambridge, MA

Riccardo Comin is an Assistant Professor of Physics at MIT, leading the Photon Scattering group. For the last 8 years, Riccardo has been using photoelectron spectroscopy and x-ray scattering techniques to shed light on quantum electronic phases of matter in correlated electron systems. His current research combines the synthesis of new transition metal-based compounds with the development and use of new coherent x-ray tools to advance our understanding of the nanoscale texture of electronic orders in quantum materials. In addition to pursuing the unprecedented opportunities in coherent x-ray science unlocked by the NSLS-II facility, Riccardo is engaged in fostering new collaborations and partnerships between the academic materials research community and BNL.

Matt Dawber
Stony Brook University
Stony Brook, NY

Matt Dawber is an Associate Professor in the Department of Physics and Astronomy at Stony Brook University. His research focuses on ferroelectric oxide materials and he runs parallel programs of synthesis and characterization of artificially layered epitaxial thin films in his lab at Stony Brook and the NSLS-II and CFN facilities at BNL. His principal interests in x-ray scattering are surface x-ray diffraction, particularly in-situ during film growth or under applied electrical field, and as such he is part of a Partner User group at the ISR beamline to develop and support a facility for in-situ x-ray diffraction during the growth of oxide thin films. He is interested in finding ways to help users be productive as possible as they gain access to the rapidly increasing capabilities available at NSLS-II.
Nominees for the 2017-19
NSLS-II Users’ Executive Committee

Mark Dean
Brookhaven National Laboratory
Upton, NY

Mark Dean is an Associate Physicist in the X-Ray Scattering Group at Brookhaven. His research program is centered on resonant elastic and inelastic x-ray scattering studies of correlated oxide materials and is supported by a Department of Energy Early Career Award. Mark was a member of the BAT for the SIX beamline and has served as Chair of the Inelastic Scattering Proposal Review Panel at the Advanced Photon Source. His priority, if elected, is to support the communities’ efforts to perform groundbreaking new experiments exploiting the source properties and new instrumentation at NSLS-II.

Miguel Garcia-Diaz
Stony Brook University
Stony Brook, NY

Dr. Garcia-Diaz is an Associate Professor in the Department of Pharmacological Sciences at Stony Brook University. His research on mitochondrial gene expression frequently takes advantage of x-ray crystallography and small angle x-ray scattering. He was a frequent user of the NSLS MX beamlines and participated for many years in the Rapidata MX data collection course. At NSLS-II, he was a member of the Beamline Advisory Team for the FMX and AMX beamlines. He is interested in developing a strong user community at NSLS-II and facilitating access to NSLS-II for the Structural Biology community.

Reeja Jayan
Carnegie Mellon University
Pittsburgh, PA

Reeja Jayan is an Assistant Professor in the Department of Mechanical Engineering with courtesy appointments in Materials Science and Chemical Engineering at Carnegie Mellon University. Reeja directs the Far-from-Equilibrium Materials Laboratory (FEMLAB) at Carnegie Mellon. Her work investigates the use of electromagnetic fields to synthesize materials that can access regions of the phase space diagram, which are difficult to access under conventional methods. Her group has been a regular user of the XPD beamline at NSLS-II and is currently setting up in-situ microwave assisted synthesis reactor at the beamline for studying materials for energy storage. She is interested in establishing and facilitating access to more in-situ, in-operando user facilities at NSLS and NSLS-II.
Nominees for the 2017-19
NSLS-II Users’ Executive Committee

Hilmar Koerner
Air Force Research Laboratory
Wright-Patterson AFB, OH

Hilmar Koerner is a Research Chemist at the Air Force Research Laboratory at Wright-Patterson Air Force Base, Ohio, working in the Polymer Matrix Composites research team. Hilmar has been a longtime synchrotron beamline user carrying out research at SAXS beamlines at CHESS, NSLS and ALS working on a number of different projects related to structure and morphology evolution within liquid crystal polymers/thermosets, nanocomposites, nanoparticle growth and photovoltaics. His recent focus is on the development of higher temperature polymer thermosets, hybrid matrix materials and their additive manufacturing and applying scattering techniques to understand processing-structure-property relationships and advance the performance of these systems. He is interested in improving awareness of NSLS-II capabilities for Air Force Research Lab researchers and increase their participation.

Amy Marschilok
Stony Brook University
Stony Brook, NY

Amy C. Marschilok is currently a Research Professor and University Instructional Specialist in the Departments of Materials Science and Engineering and Chemistry, and Center Operations Officer for the Center for Mesoscale Transport Properties (m2m EFRC) at Stony Brook University. Her current research goals center on development and investigation of new material and electrode concepts for high power, high energy density, extended life primary and secondary electrochemical energy storage systems; and understanding and controlling electrochemically mediated reactivity in functional systems. She and her research group are frequent NSLS-II and CFN users, and their research effort has been elevated significantly through productive collaborations with several BNL scientists. She would welcome the opportunity to serve the vibrant user community at BNL.

Scott Misture
Alfred University
Alfred, NY

Misture received his BS and Ph.D. degrees from Alfred University, followed by an additional 1 year of study at the Siemens Corporate Research labs in Munich and ~2 years at Oak Ridge National Laboratory. His expertise is in the area of structure-property relations in electrically active oxides, primarily for energy conversion. Misture uses advanced in-situ structural characterization tools to understand the effects of structure at the atomic and
Nominees for the 2017-19
NSLS-II Users’ Executive Committee

Stan Petrash is a Scientific Principal at Henkel Corporation, heading Advanced Characterization Group within Henkel’s Materials Science & Engineering R&D platform. Stan conducts both open and proprietary research using an extensive international network of governmental and academic user facilities, with a specific focus on synchrotron light sources in US (NSLS, NSLS-II, ALS, SSRL) and Europe (ALBA, SLS, ESRF). Stan is also a Visiting Researcher at Princeton University and has recently been selected as Henkel Technologist-in-Residence at Brookhaven National Lab. Stan is striving to promote and develop close, mutually-beneficial collaborations between synchrotron scientists and industrial researchers.

Michael Pierce is an assistant professor of physics at Rochester Institute of Technology in upstate NY, and has been an x-ray synchrotron user for over 15 years. Prior to joining RIT he was a post-doc and assistant physicist at Argonne National Laboratory in the Materials Science Division. He has diffraction and scattering experience at several x-ray facilities around the country including NSLS-II, APS, and ALS. Prof. Pierce has participated on several DoE service committees, including the Advanced Photon Source User Organization Steering Committee and as a regular panelist for the APS condensed matter physics proposal review panel. He has also served in different capacities on panels and collaborated on beamline upgrades/proposals at both APS and NSLS-II. His research focuses on surface science, phase transitions, and magnetic systems, all studied through synchrotron based x-ray scattering.

Misture has published some 150 refereed papers and has given over 300 presentations. Misture serves the materials science community as a principal editor of the Journal of Materials Research, as immediate past Chairman of the Board of Directors of the International Centre for Diffraction Data and as past Chair of the Basic Science Division of the American Ceramic Society.