NSLS-II Beamline Report for SAC Review of Beamlines

Beamline: ***Sub-micron Resolution X-ray Spectroscopy (SRX) Beamline, 5-ID***
Report Date: March 27, 2019

Introduction

Scientific communities such as geo- and environmental sciences, medical and life sciences, condensed matter and material sciences, chemical and energy sciences, have identified the need for a high intensity X-ray microprobe to advance the understanding of complex natural and engineered systems that are heterogeneous on the µm to the sub-µm scale. Beamline 5-ID, the Sub-micron Resolution X-ray Spectroscopy (SRX) beamline, with its unique combination of high spectral resolution over a very broad energy range and very high beam intensity in a sub-µm spot, is a tool very well suited for the characterization of these systems, in terms of elemental abundances and speciation. It has been designed, installed and commissioned as an X-ray fluorescence analytical probe dedicated to spectroscopy experiments with sub-µm spatial resolution. X-ray fluorescence (XRF) mapping and X-ray absorption near-edge structure (XANES) spectroscopy experiments to investigate the elemental composition and the chemical state of a sample are the core capabilities of this beamline. The scientific emphasis is the study of complex systems with chemical heterogeneity at sub-µm length scales. The photon flux of 10^{12-13} phot/sec that SRX delivers in a sub-µm spot opens up new possibilities for compositional and spectroscopic analysis of major and trace elements in natural and synthetic materials. The accessible energy range of 4-20 keV allows for X-ray absorption spectroscopy experiments across the periodic table from titanium up to plutonium. In order to meet scientific demands for higher resolution and multimodal imaging, the development of additional capabilities is underway. A new nano-KB system with a resolution down to 100 nm is under construction, to be installed in late 2019. In addition, multimodal imaging capabilities are being commissioned, in order to visualize local morphology through differential phase contrast and crystalline phases through microdiffraction, simultaneously with elemental mapping through X-ray fluorescence. X-ray fluorescence tomography will allow mapping of the elemental composition of samples down to trace elemental levels in 3D. The SRX beamline was developed as one of the seven project beamlines at NSLS-II, funded through Basic Energy Sciences (BES).

The SRX Beamline received the first synchrotron light on Dec 08th, 2014, X-ray fluorescence mapping and XANES spectroscopy in spring 2015, and performed first user experiments (as commissioning users) in June 2015. SRX received an approval for general user operation in November 2015. The general user program has been ramped up since then showing a beam time usage of ~65%.

SRX Beamline Overview

Originally, SRX was designed as a two-branch beamline for high quality sub-µm resolution spectroscopy. The configuration requires beamline to make use of two undulators, one for each branch, in a canted geometry on a short (low-beta) straight section. The first branch is optimized to cover the energy range from 4.65 to 20 keV. Mirror optics in the Kirkpatrick–Baez (KB) geometry focus the beam and create a sub-µm sized focal spot. This branch is the current SRX beamline. The second

branch, optimized for lower energies and accessing spectroscopic edges from 2 to 12 keV, was designed to use zone plates optics to focus the beam below 30 nm. The two branches are required to cover this large energy range without compromising the goal of combining sub-µm spatial resolution and X-ray spectroscopy in an optimal way. The optical scheme of the whole beamline is shown in Figure 1. The second branch still requires additional funding to be completed. Only the hutch has been installed, leaving room for a future endstation instrument. Only one undulator, an in-vacuum device with 21 mm magnet period (IVU21), has been installed, serving the first branch. On the other hand, the existing front end and the optical components in 5-ID-A were designed and installed to accommodate a future insertion device at a canting angle of 2 mrad.

Apart from a couple of fixed masks and white beam slits upstream, the first optical component of SRX is a 1 m long horizontal focusing mirror (HFM) at 34 m distance from the IVU21 undulator. It is followed by pink beam slits and at 36 m by a double crystal monochromator (DCM), designed to deflect horizontally for high stability. In addition, the horizontal diffraction geometry also increases the separation distance between the two branches. The HFM creates an image of the undulator source in the horizontal plane at the secondary source aperture (SSA) at 51 m. This image is the source point for the horizontally deflecting KB mirror located downstream, whereas the vertically deflecting KB mirror is looking at the primary source in the undulator. The KB mirrors, positioned at about 65 m, produce a de-magnified image of these source points at their common focal spot. A variety of detectors are available for fluorescence, transmission, differential phase contrast and diffraction measurements.

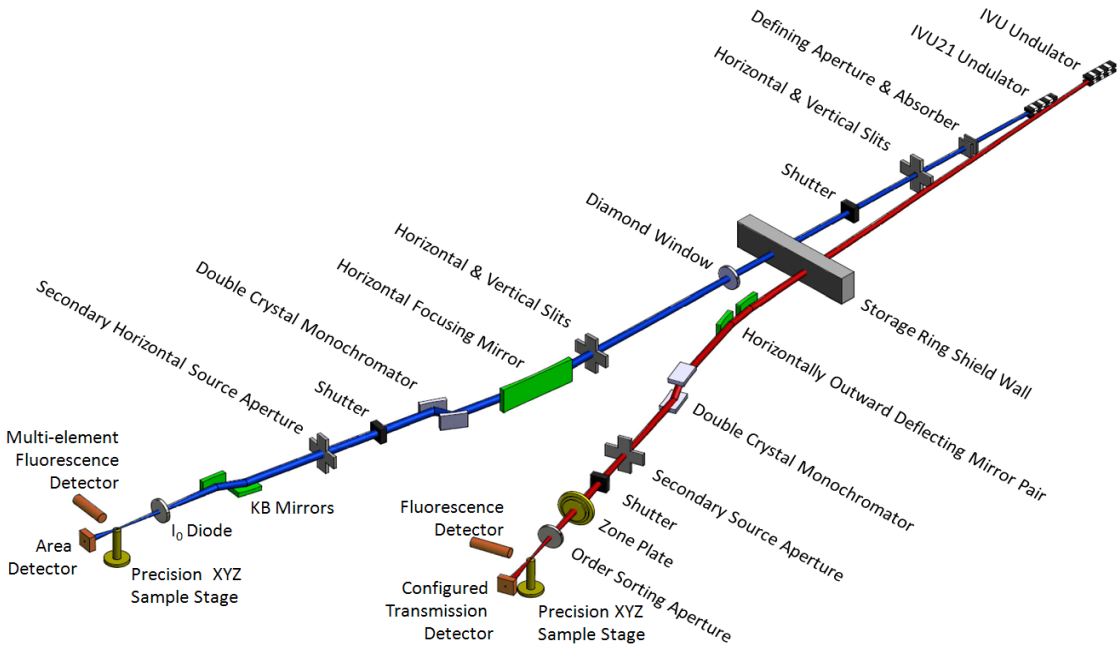

Figure 1: Schematic view of the major optical components of the Sub-micron Resolution X-ray Spectroscopy Beamline. The branch laid out in red has not been built out.

Staff

Currently, the SRX beamline is supported by the following labor efforts:

- Yong Chu (~0.25 FTE, lead beamline scientist/program manager)
- Andrew Kiss (1 FTE, beamline scientist)
- Yang Yang (1 FTE, beamline scientist, starting May 2019)
- Juergen Thieme (0.5 FTE beamline scientist; 0.5 FTE as science coordinator)
- Randy Smith (0.5 FET, scientific associate)
- Petr Ilinski (0.3 FTE, scientific associate)

In addition, the beamline receives matrixed software engineer and mechanical engineer support. Two technicians and two scientific associates are shared within the I&M program, supporting five beamlines.

It should be mentioned that SRX had quite a turnover in staff since it was first built, which made the installation and commissioning of the beamline a difficult task. After the design phase, beamline scientist V. deAndrade left NSLS-II in January 2015, requiring the lead beamline scientist J. Thieme to work on his own for several months to complete beamline installation and instrument readiness validation. K. Chen-Wiegart joined SRX in the summer of 2015, first as a postdoc, then as a beamline scientist. A couple of months later G. Williams joined the SRX staff. During his work for SRX, G. Williams has invested much of his time developing scan routines, making data acquisition possible and creating workflows for user operations. In January 2017, K. Chen-Wiegart transferred to a position as an Assistant Professor at Stony Brook University. The effort by G. Williams was ramped down during the period from Sept 2017 to April 2018, so that could take leadership of developing the upcoming Bragg-CDI beamline. There was a period from Sept 2017 through Jan 2019, where the ownership of the fly-scanning at the SRX beamline was not fully taken up by the DAMA. During this period, the data collection through the fly-scanning mode was not stable and created considerable negative impact to the user operation.

J. Thieme took on the new function as science coordinator in the summer of 2017, while Y. Chu took over the lead beamline scientist role. In January 2018, A. Kiss joined the SRX beamline, and in May 2019, Y. Yang will start as a beamline scientist, restoring the adequate level of beamline scientist effort for operating the SRX beamline.

Beamline Mission

The SRX beamline attracts users from many different science areas, including earth, planetary, and geoscience (22.5%), energy research (18.1%), material science (15.5%), environmental science (13.8%), bioscience (9.5%), and others. About one third of the user community consists of experienced, returning users, who are able to run experiments with basic support at the beamline and whom we support just for beamline setup and preliminary data analysis. Two thirds of the users, however, will need support all the way from proposal writing and preparation of the experiment to the actual measurements, the data analysis and the preparation of a publication. This has several reasons. New user groups naturally need full support of the beamline staff to have a productive beamtime. However, even returning, larger user groups need support since postdocs and graduate students change constantly. Thus, new users are constantly introduced and trained for procedures at the beamline, as

well as assisted with data analysis using the XRF analysis program PyXRF and the spectroscopy analysis program Athena. In general, and since SRX is at the forefront of new developing scientific topics, support will always be required. Increasingly, users asked for the availability of higher spatial resolution as well as additional techniques such as tomography, differential phase contrast imaging and microdiffraction. These requests can be fulfilled based on future developments at SRX. Considering the actual plans for further development of SRX, all these requests can be addressed in the near future. The number of submitted general user proposals has decreased in the last cycles. It is foreseeable that these numbers will increase again when beamline staffing is complete and all requested techniques are available. This will be associated with an increase in the percentage available for general user time.

In addition to the standard provisions directly at the beamline, significant ancillary capabilities exist for user operations. The Mesoscale Imaging Wet Lab provides a suite of optical microscopes and bio-sample preparation methods. The Environmental Wet Lab provides a range of support for handling and preparing bio/geo/soil samples, including a glove box for the handling of anoxic samples. The Chemistry Wet Lab has a glove box for assembling battery cells or handling Li containing samples. Due to the sample area being in air, the SRX beamline offers for users the possibility, to study samples in-situ or in an operando case without great complications. Specialized sample holders for specific, recurring samples have been designed and built, requests for new dedicated holders can be addressed without problem. A sample registration protocol will be developed to enable users to transfer samples from SRX to other beamlines or to come from other beamlines with a list of regions of interest to be exampled further.

All imaging and spectroscopy data are collected using BlueSky (https://github.com/NSLS-II/bluesky), which is a script-based data acquisition software developed at the NSLS-II. Despite its complexity, high-level commands are developed, so that users only need to know several commands to complete their experiment. XRF images can be extracted from the NSLS-II data broker and stored as an hdf5-file. All XRF spectra are fitted using PyXRF (https://github.com/NSLS-II/PyXRF), which provides high-speed fitting capability. Thus, the users can examine their data either using the real time element images (based on ROIs) and fitted element images immediately after the scan is completed. Software tools are available so that XANES and EXAFS spectra data can be piped into Athena (https://bruceravel.github.io/demeter/). Presently, all the data are saved to the local data storage. We plan to use the NSLS-II Central Storage, as soon as all the data transfer infrastructure is ready.

All users perform their preliminary data analysis (i.e. spectra fitting or the generation of element maps) during their beamtime and thus require initial training for data analysis. About two thirds of the users do not have sufficient expertise to perform data analysis on their own and require significant help from the beamline scientists. Software tools are available so that users convert the acquired data into a standard format (i.e. hdf5, binary, tiff, text, etc) and analyze them at home institutes.

Productivity and Impact

The SRX beamline provides a combination of X-ray fluorescence imaging with chemical sensitivity down to the ppm-levels and chemical analysis using XANES and EXAFS spectroscopy at sub-µm spatial resolution. Using XRF, elemental compositions within a sample can be determined quantitatively. Due to the versatility regarding the sample environment, many different samples can be hosted by SRX for examination, as can be seen by the series of science highlights submitted to DOE and listed hereafter. The degradation of paint pigments in paintings several centuries old has been studied using XRF imaging and XANES spectroscopy, especially aiming for the chemistry of so-called lead soaps (highlight #2). In-situ and operando studies are also possible with samples from many research areas, which is attractive for a wide range of scientific applications. Energy research, mostly the study of battery materials, is one of the larger science areas where in-situ and operando measurements with high spatial resolution have been performed at SRX. Batteries containing manganese as a new low-cost material (highlight #1), lithium-sulfur batteries (highlight #3), and nickel oxides as new electrode materials (highlight #5) have been studied under operando conditions, i.e. charging and discharging, using SRX. Materials have been investigated in-situ using sample heaters to raise the temperature up to 800 deg C while in the beamline. Another large science area is the field of earth, planetary and geo-sciences. The study of the accumulation of arsenic in plants needs the sub-µm spatial resolution to map the location of this toxic metal in the cells as well as spectroscopy to determine the oxidation state of the arsenic (highlight #4). In the light of NASA's plans to bring samples from Mars to Earth, rock samples have been investigated that can be compared in their composition to rocks from the Red Planet. During these studies, XRF maps of rocks from Greenland have been obtained, which shed a new light on structures formerly thought to be of biological origin (highlight #6). All these examples show first of all the versatility and the applicability of the SRX beamline to many scientific topics. Capabilities such as studies using high temperature and/or high pressure, in-situ and operando will be extended to be available to users with a reliable and consistent workflow. First experiments using a setup for cryogenically cooled samples have been performed, partnering with other groups at NSLS-II to develop a user-ready setup. The SRX beamline is capable of multi-modal experiments using different analytical techniques. First experiments on differential phase contrast imaging, micro-diffraction, and XRF tomography have been successfully executed. However, here as well reliable and consistent workflows need to be further developed to make these capabilities user-ready.

Science Highlights achieved at beamline 5-ID

1) Cu Insertion into Bi-Modified MnO_2 Cathodes Results in a Safe, Energy-Dense, Low-Cost Battery

Studies have shown that adding copper to bismuth-modified MnO_2 imparts high cycle life to the resulting aqueous cathode, and this benefit is maintained at high active mass loading. Bismuth-modified MnO_2 without copper, in contrast, does not remain active at the mass loadings needed to result in useful battery energy densities. The mechanism by which copper improves performance is not known. Electroanalytical testing via slow scan cyclic voltammetry suggests a complex reaction mechanism, in which species related to the interactions of the elements are apparent (for example Bi-Mn and Cu-Mn complex species). By tracking the three elements by X-ray fluorescence microscopy and micro-XANES, results showed that copper begins highly coordinated with Bi spatially (>0.95), and during initial cycling shifts to a correlation with Mn (~0.5). At the bottom of discharge, zero-valence copper is produced. This indicates that Cu^0 inserts in the Mn oxide structure, as no metallic copper was detected by XRD. Battery modeling shows that when integrated with a Zn anode, this type of electrode has the potential to establish a new paradigm in battery technology: having the volumetric energy density of Li-$FePO_4$ (200 Wh/L), with the safety of lead-acid (water-based, non-flammable), at a cost lower than both ($50/kWh capital cost).

Yadav, Gallaway, Turney, et al., Nature Communications, 8:14424, 1-9 (2017)

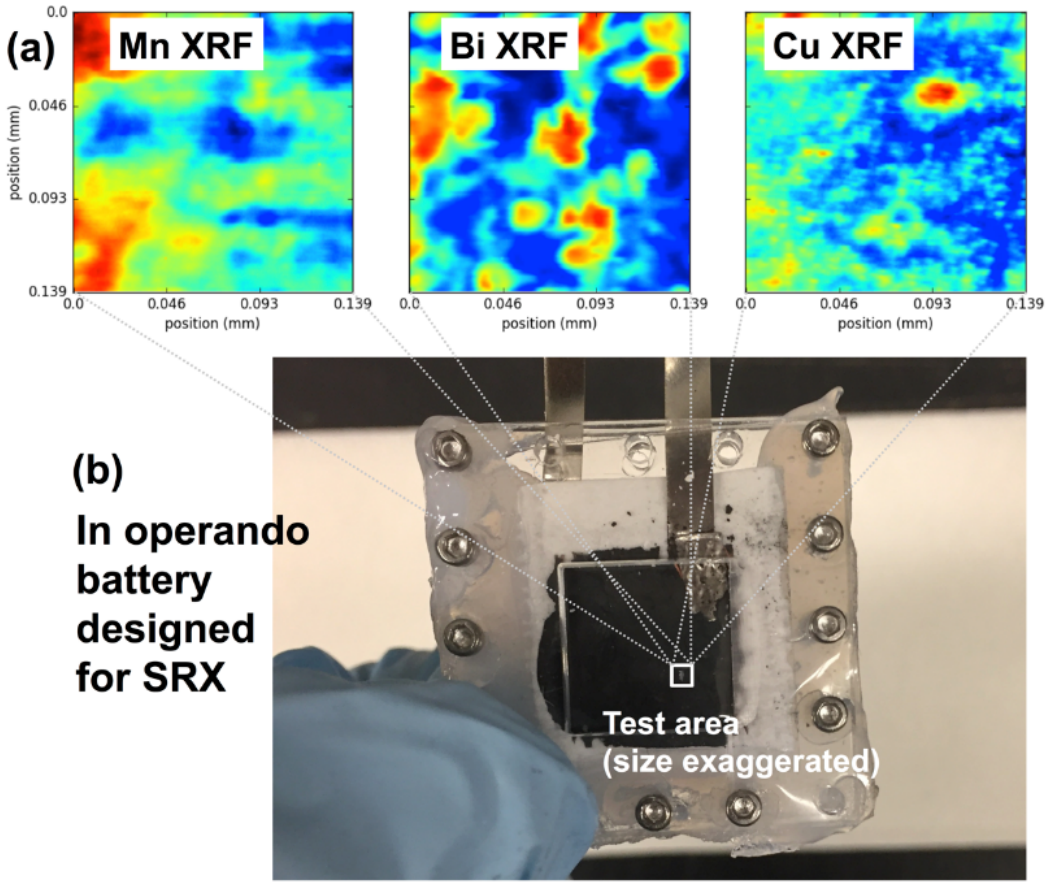

Figure 2: *(a) X-ray fluorescence microprobe imaging of Mn, Bi, and Cu in the battery cathode. (b) Photography of the test battery designed for the SRX beamline at NSLS-II.*

2) Shedding (X-Ray) Light on 15th Century Oil Painting Degradation

One major degradation factor in oil paintings is the soap formation of heavy elements. This chemical process is a serious challenge for preservation efforts because its underlying mechanisms are not well understood. The process is linked to the environmental conditions of the painting, but how to arrest or prevent the formation of soaps is so far unknown. It is theorized that free fatty acids in the oil binding mediums move through the paint and react with pigments containing heavy metals to form these soaps. To improve preservation efforts, beamline 5-ID at NSLS-II has been used to combine X-ray fluorescence microscopy and absorption spectroscopy techniques to shed light onto the chemical process of soap formation in oil paintings. This study demonstrates the usefulness of modern X-ray microscopy and spectroscopy methods to characterize the chemical conditions of a paint sample from a 15th century painting degraded by soap formation. It shows the distribution of lead soap in the sample and other chemical components correlated with the degradation process.

Chen-Wiegart, Catalano, Williams, et al., Scientific Reports, 7:11665, 1-9 (2017)

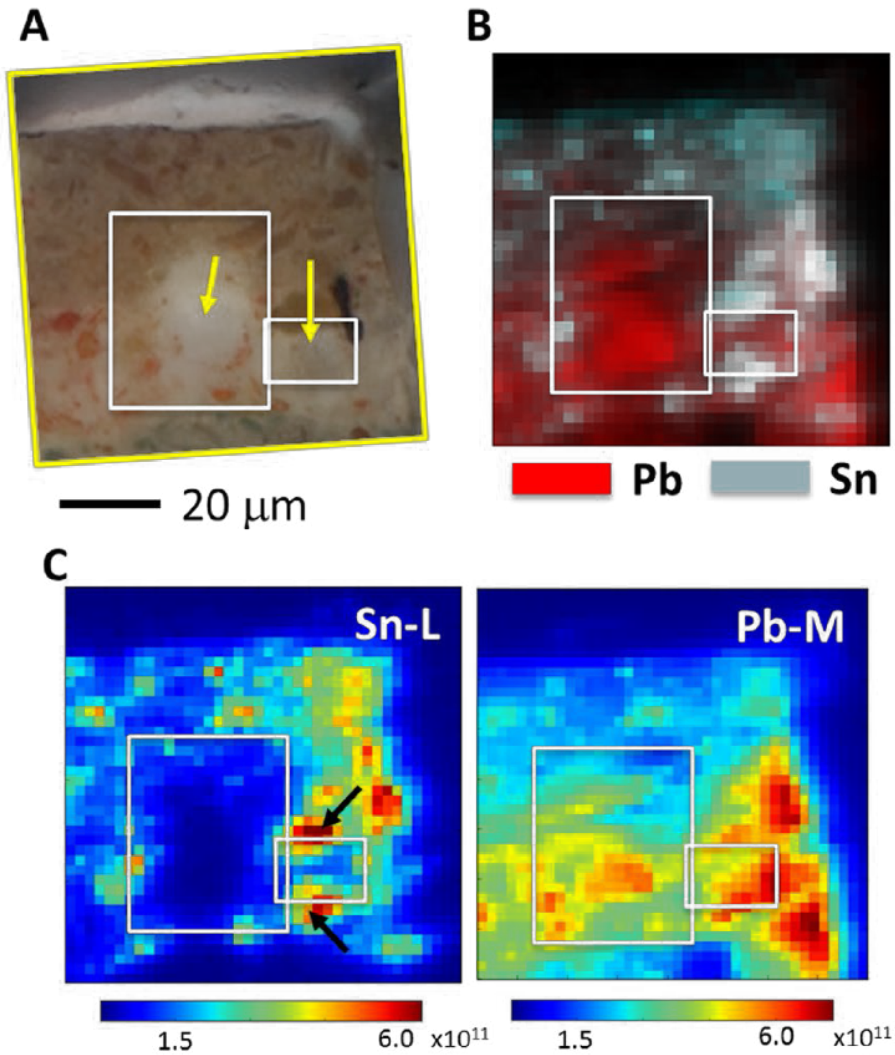

Figure 3: *The same spot in the painting sample seen with different techniques:*
A) is a photomicrograph image while B) and C) show x-ray maps of the location of lead and tin within the sample.

3) Multimodal Approach Provides Insight into Lithium-Sulfur Batteries

A multimodal approach has been employed successfully to study a new type of lithium-sulfur battery and to give a new description of the battery's chemistry. Lithium-sulfur batteries with conductive metal sulfides as multi-functional additives are promising new electrochemical energy storage devices but their fundamental chemistry needs to be understood before they can be used as batteries. The additives that improve the batteries capacity, can pose additional challenges such as parasitic chemical reactions. Studying such complex reactions presents a challenge because the scientists need experimental methods that can track the chemical and structural evolution of the system during an electrochemical process. Various X-ray characterization techniques have been used that offer complementary insights into the chemical reactions and possible side effects of these batteries. X-ray powder diffraction, X-ray fluorescence imaging, and X-ray absorption spectroscopy were used to resolve the different stages of the reaction during lithiation and de-lithiation of a Li-S battery with CuS as the multifunctional cathode additive. With these complementary techniques crystalline phases, amorphous phases and the elemental distribution have been identified. The dissolution mechanism has also been described: The lithiation of CuS starts at the very end of discharge to form amorphous Cu1+xS. During this process, CuS interacts strongly with soluble low-order polysulfide species. The dissolved Cu ions then migrate to the anode side and alter the anode SEI, causing the fast capacity-fade.

Sun, Zhao, Lin, et al., Scientific Reports, 7:12976, 1–10 (2017)

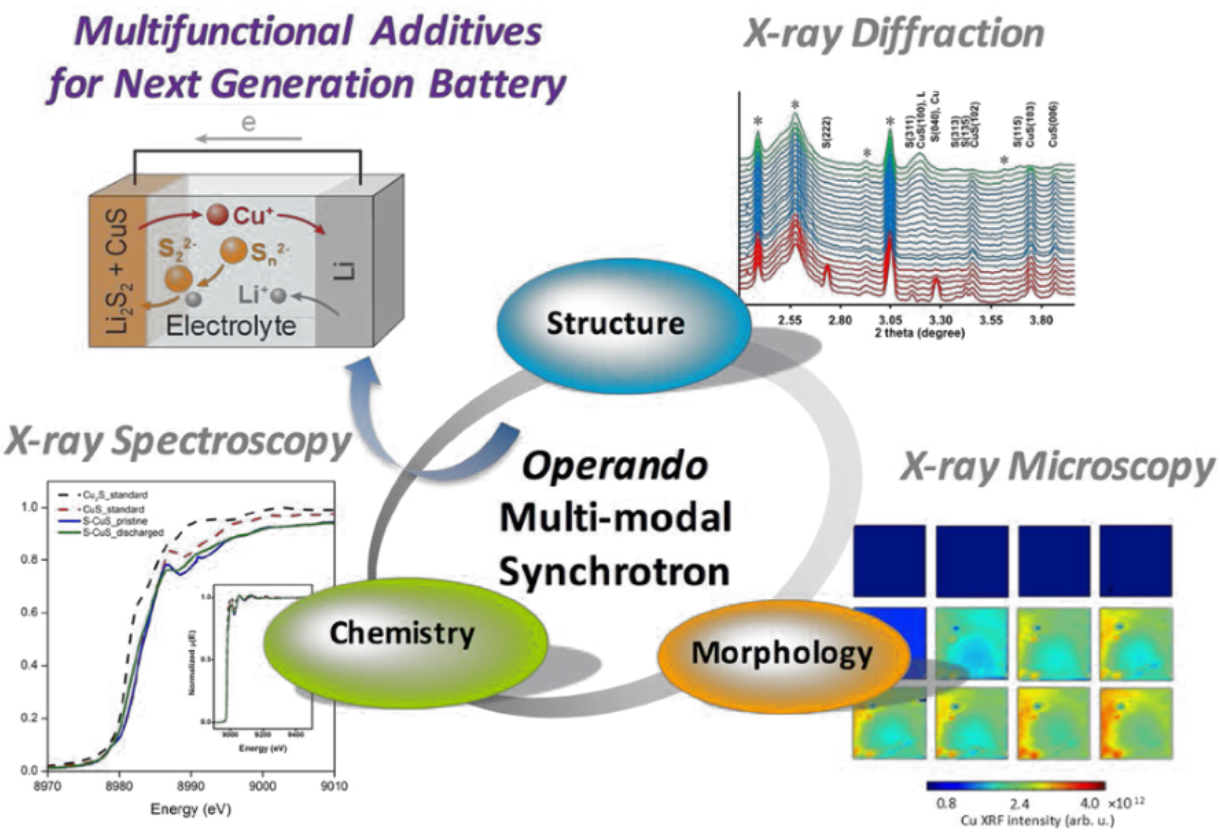

Figure 4: *To fully understand the fundamental behavior and the reaction mechanisms of lithium-sulfur batteries with S/CuS hybrid electrode, the scientists used three different synchrotron techniques to study the chemistry, structure and morphology of the battery.*

4) Using Plants to Immobilize and Stabilize Arsenic in the Soil

Phytostabilization is a cost-effective long-term bioremediation technique for the immobilization of metalliferous mine tailings. However, the biogeochemical processes affecting metal(loid) molecular stabilization and mobility in the root zone remain poorly resolved. The roots of *prosopis juliflora* grown for up to 36 months in compost-amended pyritic mine tailings from a federal Superfund site were investigated by microscale and bulk synchrotron X-ray absorption spectroscopy (XAS) and multiple energy micro-X-ray fluorescence imaging to determine iron, arsenic, and sulfur speciation, abundance, and spatial distribution. Whereas ferrihydrite-bound As(V) species predominated in the initial bulk mine tailings, the rhizosphere speciation of arsenic was distinctly different. Root- associated As(V) was immobilized on the root epidermis bound to ferric sulfate precipitates and within root vacuoles as trivalent As(III)−(SR)3 tris-thiolate complexes. Molar Fe-to-As ratios of root epidermis tissue were two times higher than the 15% compost-amended bulk tailings growth medium. Rhizoplane-associatedferric sulfate phases that showed a high capacity to scavenge As(V) were dissimilar from the bulk-tailings mineralogy as shown by XAS and X-ray diffraction, indicating a root-surface mechanism for their formation or accumulation.

Hammond, Root, Maier, Chorover: Environmental Science and Technology, 52(3), 1156–1164 (2018)

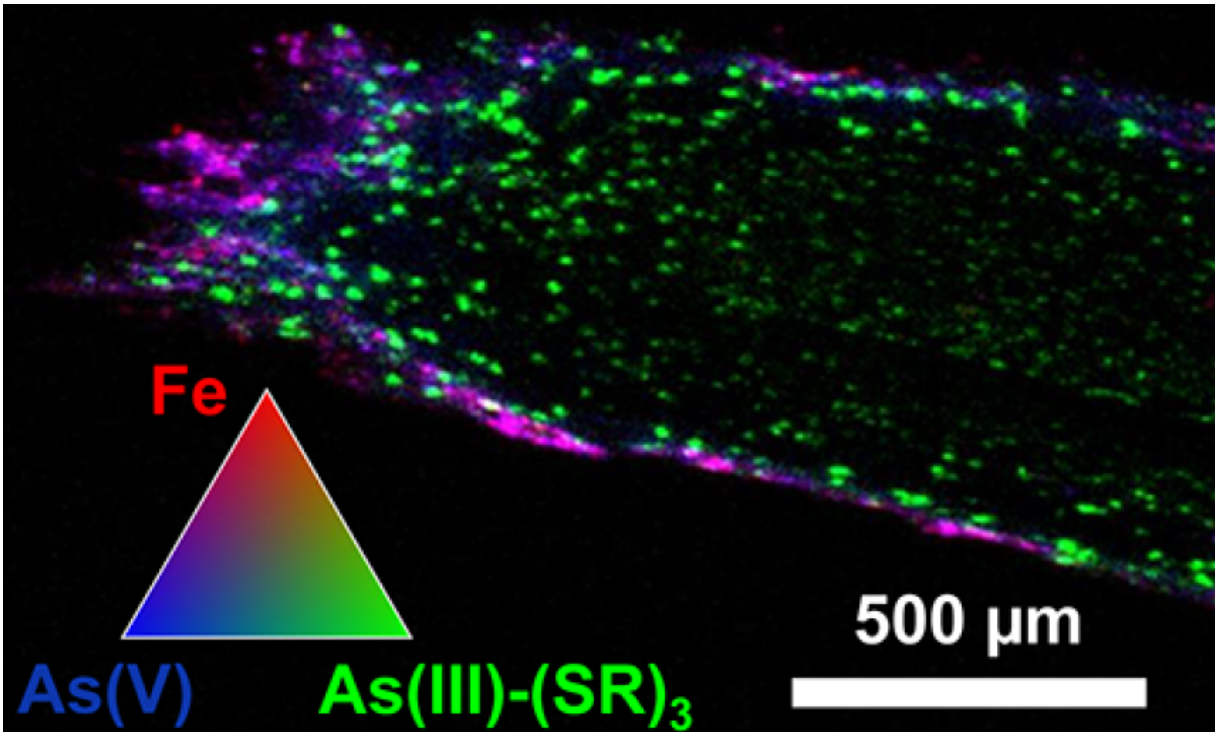

Figure 5: *Microscale x-ray fluorescence imaging of a 30 µm thick P. juliflora root thin section from a plant grown at the IKMHSS tailings amended with 15% compost and lime for one year. The tricolor plot represents an overlay of Fe, As(V), and As(III)−S in a 10:1:1 ratio of intensity scales.*

5) New Insights into the Synthesis Process of Layered Oxides

Metal (M) oxides are one of the most interesting and widely used solids, and many of their properties can be directly correlated to the local structural ordering within basic building units (BBUs). One particular example is the high-Ni transition metal layered oxides, potential cathode materials for Li-ion batteries whose electrochemical activity is largely determined by the cationic ordering in octahedra. In this study, a multimodal in situ X-ray characterization approach has ben used to investigate the synthesis process of a specific transition metal layered oxide (LiNi0.77Mn0.13Co0.10O2) from its hydroxide counterpart, at scales varying from the long range to local individual octahedral units. To study this material a combination of x-ray diffraction (XRD), pair distribution function (PDF) analysis and x-ray absorption near-edge spectroscopy (XANES) at multiple NSLS-II beamlines (28-ID-2 and 5-ID) as well as beamlines at the Cornell High Energy Synchrotron Source has been used. The study shows how defects in the structure effect the performance of these materials as battery cathodes.

Zhang, Teng, Chen-Wiegart, Duan, et al., JACS, 140(39), 12484–12492 (2018)

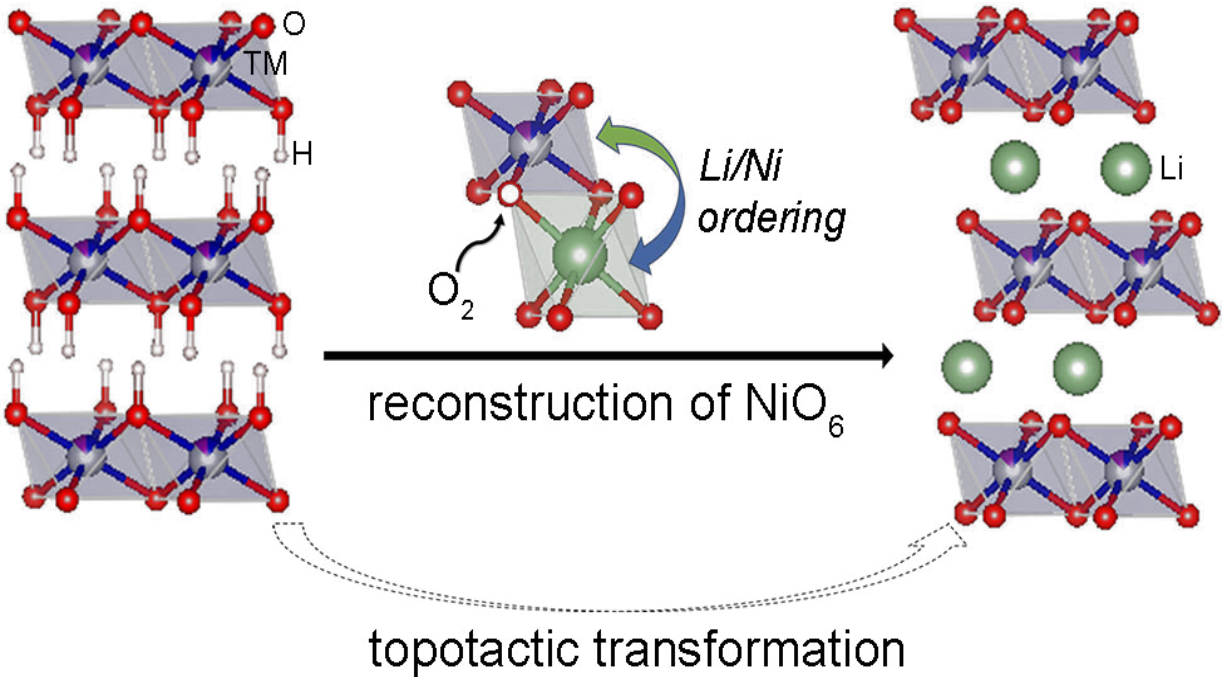

Figure 6: *By using a combination of in situ x-ray characterization techniques at NSLS-II beamlines 28-ID-2 and 5-ID, scientists investigated the structural evolution of a transition metal layered oxide during its synthesis. Their new insights helped them to understand how the layers arrange on larger and smaller scales.*

6) 3.7 Billion Year Old Structures Formed by Tectonics, not Life

In this study, the evidence of life in 3.7-billion-year-old rock structures has been re-examined. The result was that the structures were of geological origin and not as previous thought of biological origin. Until this recent new study, the structures were considered the earliest evidence for life on Earth. Finding evidence and dating the first beginnings of life on Earth has important implications for the understanding on how life emerged and evolved on Earth. This knowledge can also help scientists for the search of life on Mars or other planets. The previous studies on these rock samples employed millimeter scale information using laser ablation analysis to determine the origin of the formations. For this new study X-ray florescence microscopy at SRX with a 1 µm focal spot at the NSLS-II has been used. Using SRX, crucial new evidence based on the elemental make-up of the rock structures ahs been revealed. This evidence supported the conclusion that the rock formations are of non-biological origin. Allwood, Rosing, Flannery, etal., Nature 563, 241–244 (2018)

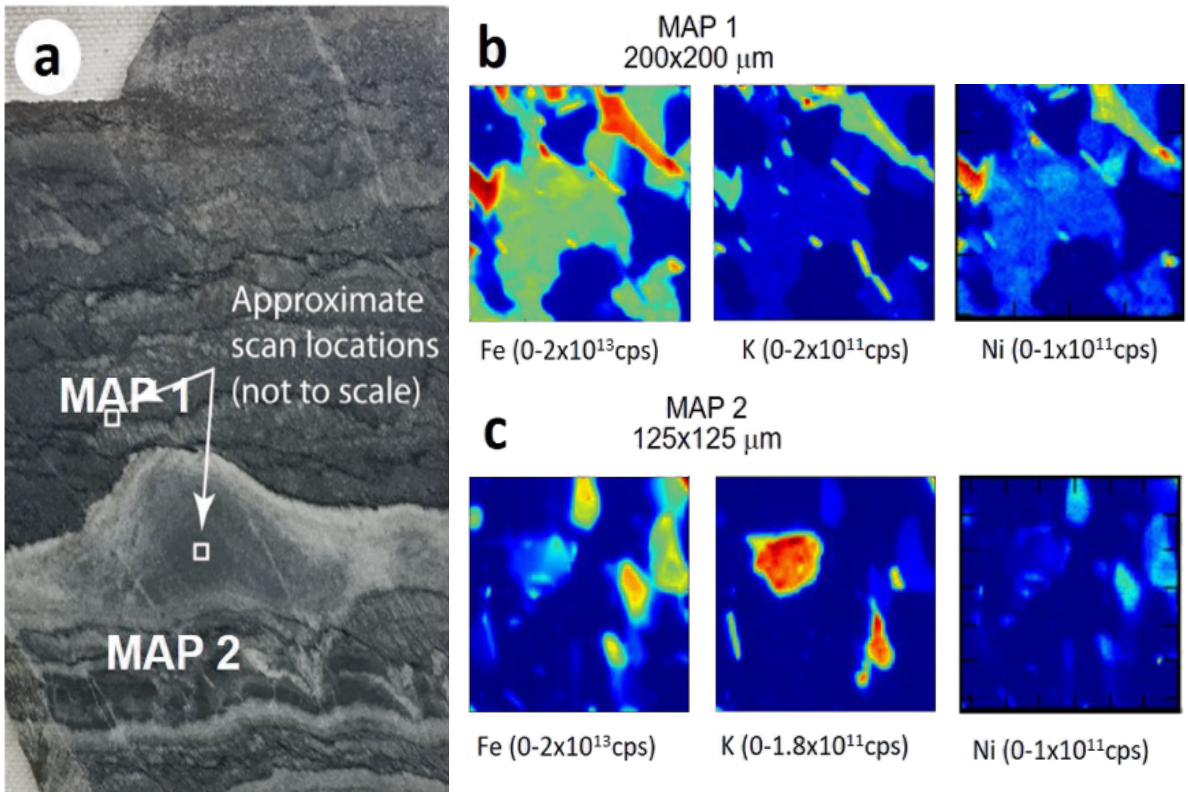

Figure 7: *Image a) shows a photograph of the rock sample, while the collection of x-ray images b) and c), obtained at SRX beamline 5-ID, show the elemental distribution of the indicated regions in image a). These chemical maps reveal fine-scale chemical and mineralogical variations that were not captured in previously published analyses.*

Vision for Next Five Years

The SRX beamline aims to achieve imaging and spectroscopy capabilities with higher spatial resolutions in 2D and 3D, with provision for multimodal imaging capabilities such as phase contrast and microdiffraction. We aim to achieve higher measurement throughput and scientific productivity by offering robust and reliable workflows for user experiments. In order to achieve this vision, we plan the following developments and upgrades.

- Robust Spectromicroscopy capabilities from 0.1 to a few µm spatial resolution, supporting users from a broad range of scientific disciplines. A new nano-KB mirror system will be installed by the end of 2019, allowing for improved spatial resolution. We will begin technical commissioning in early 2020, followed by science commissioning in collaboration with the experience user groups (i.e. through science commissioning proposals). We plan to offer this capability to general users either in late 2010 or early 2011.

- Develop a range of in-situ capabilities by taking advantage of the larger working distance of SRX (several centimeters in comparison with a few millimeters for the HXN or the FXI beamline). As described in the preceding text, significant efforts have been already made for investigating energy storage materials under in-situ conditions. In-situ heating has been tested for the study of nickel oxides as well as for molten salt investigation, in support for the Molten Salt EFRC project at BNL. In addition, possibilities will be explored further for performing in-situ high-pressure experiments using a diamond anvil cell (DAC) adapted to the sample environment of the SRX beamline.

- Enable multimodal imaging capabilities including microdiffraction and differential phase contrast imaging. These techniques and the analysis workflow have been already implemented at the HXN beamline. At the SRX beamline, both, microdiffraction and differential phase contrast imaging, are being commissioned and will provide a more comprehensive analysis capability, which is important for instance for material science, geochemistry, and high-pressure science.

  Expanding XRF imaging into the third dimension using conventional XRF tomography. This is the most suitable technique to investigate in the best possible way complex samples with a heterogeneous internal structure. Using the penetration ability of high energy X-rays in combination with the detection limits in the ppm range for X-ray fluorescence, XRF tomography can shed light on porous materials, on cracks and fissures, and on the emergence of segregation in previously homogeneous samples. This is for example of utmost importance in energy research, where mixtures of battery materials influence the performance, or in geosciences, where porosity can be a determining factor in material transport. The XRF-tomo workflow (data collection to analysis) has been developed at HXN and will be transported to the SRX beamline. An additional path to obtain 3D-information from samples to thick to penetrate is the use of confocal X-ray fluorescence microscopy. Presently, we are collaborating with the researcher from CHESS using the channel array collimator (CAC). In addition, we plan to achieve this capability using a single-bounce capillary optics. We submitted a funding proposal to DOE-BER to gain resources (materials and labor).

- To enable thorough bioscience experiments, it is necessary to be able to handle samples in a cryogenically cooled state. First experiments at the SRX beamline have been carried out successfully. However a complete workflow will be a pre-requisite for comprehensive studies. Across the beamlines of the imaging and microscopy program (FXM and TES), tests and experiments will be carried out in this regard, experiences will be shared. A funding proposal to DOE-BER has been submitted to gain external resources (materials and labor).

Beamline Self-Assessment

The strength of the SRX beamline lies, inter alia, in its flexibility and versatility. Multimodal measurements on a sub-µm size scale are a core capability. This spatial resolution connects the use of micro-probes such as TES or XFM with experiments at HXN, therefore enabling user science across all length scales at NSLS-II. The beamline staff shows expertise in material science, energy research, and geo-sciences, thus being able to support a wide range of user communities optimally. For that reason, further growth in these science areas is expected. The beamline allows for XAFS spectroscopy with high spatial resolution, XANES spectroscopy is a routine measurement and first EXAFS measurements have been published. At present, the already described problems with SRX's monochromator affect these capabilities negatively. An improved monochromator would of course boost spectroscopy significantly. To work with biological samples, handling of frozen hydrated samples is a basic prerequisite. An excellent way to fulfill these requirements would be to equip the second branch of the SRX beamline with an X-ray microscope dedicated to the study of cryogenically cooled samples. This was conceived in the original plans, but has not received funding yet.

Supplement Information: SRX Beamline User Statistics

The beamtime usage is defined as the fraction of the beamtime allocated for user experiments, which includes general users, science commissioning users, and beamline staff users.. Figure SI-1 shows these data in a graphic representation, separating between user time and technical commissioning time. Figure SI-2 shows the number of submitted proposals in comparison to the allocated proposals. Table SI-1 summarizes the beamline users by cycle and year. The scheduled beamtime can then be categorized by scientific discipline with beamtime allocated to material science (15.5%), energy research (18.1%), environmental science (13.8%), Earth/Planetary/Geoscience (22.5%), bioscience (9.5%), instrumentation development (7.7%), nuclear science (5.2%), education (5.2%), proprietary (0.9%), and cultural heritage (0.9%). Figure SI-4 summarizes the allocated beamtime distributions to different scientific disciplines.

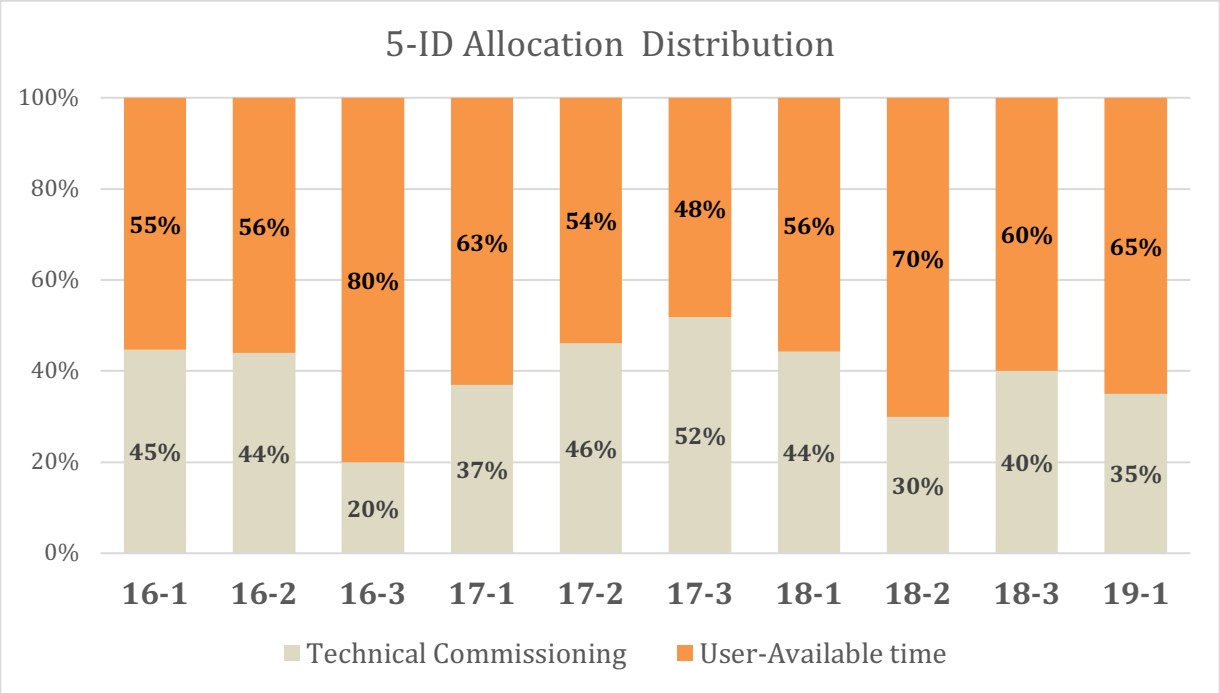

Figure SI-1: Percentage of beamtime at 5-ID allocated to technical commissioning and user time

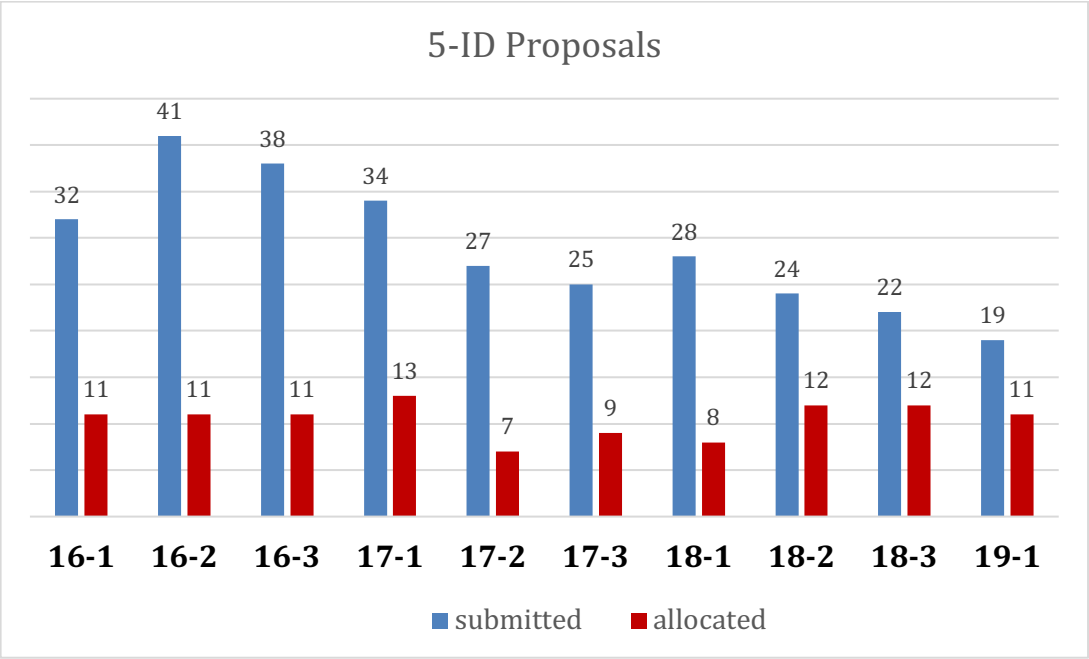

Figure SI-2: Submitted and allocated proposals from 1st cycle of 2016 to 1st cycle of 2019

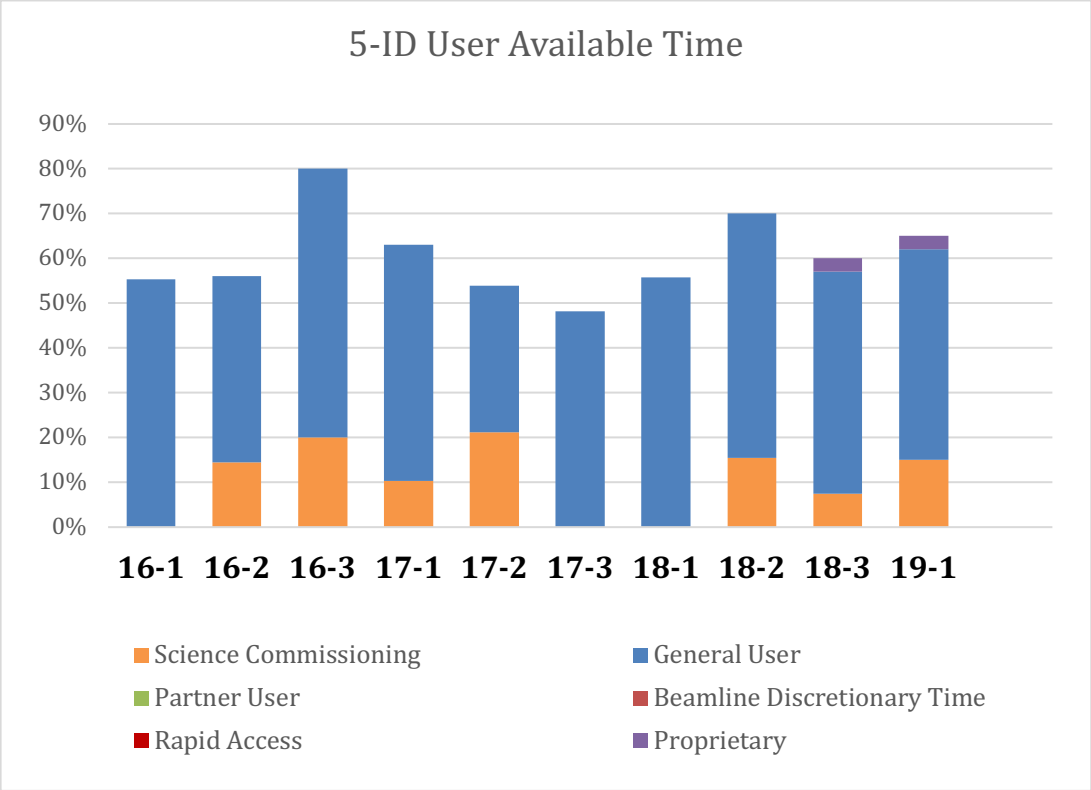

Figure SI-3: Segmentation of time available for users into General User Time, Science Commissioning Time and Proprietary Time. All other options did not occur at 5-ID.

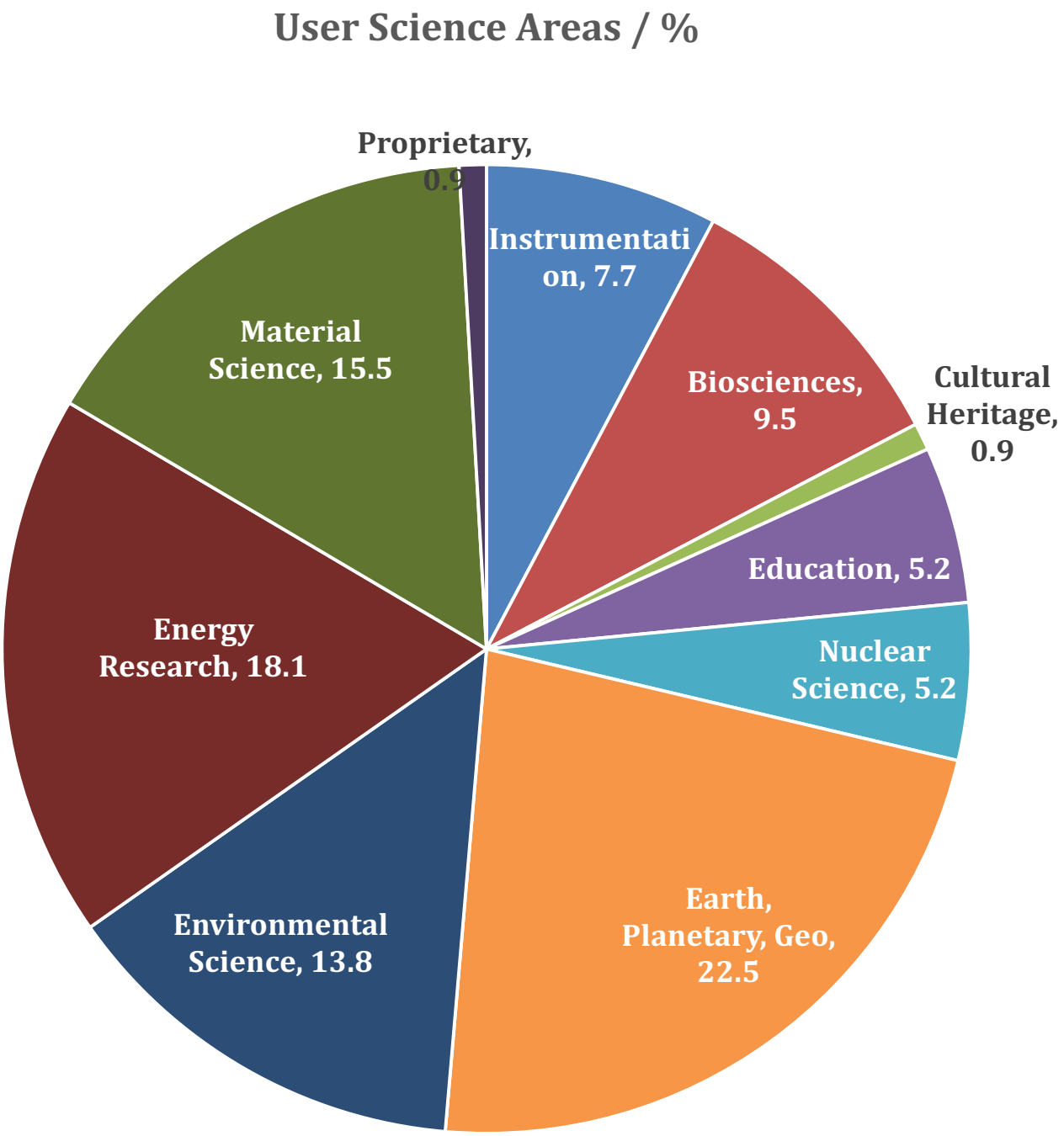

Fig. SI-4: Segmentation of available user time at 5-ID into science areas, following table SI-1.

Table SI-1: Complete list of the allocated general user proposals by principal investigator and beam cycle

Cycle	Last Name	First Name	Shifts	Science Area	Affiliation
19-1					
	Bock	David	9	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Chou	Kang Wei	9	Material Science	Henkel Corporation, Duesseldorf, Germany
	Miller	Lisa	12	Bioscience	BNL
	Pactunc	Dogan	12	Environmental Science	CANMET Ottawa, Canada
	Schlesinger	Danielle	9	Environmental Science	Princeton University, Princeton, NJ
	Tenzer	Selina	12	Earth Science	Friedrich-Schiller-University, Jena, Germany
	Trewhella	Catherine	12	Planetary Science	University of Massachusetts, Amherst, MA, and BNL
	Turney	Damon	15	Energy Research	City College of New York, New York, NY
	Wang	Feng	9	Energy Research	BNL
	Woll	Arthur	15	Instrumentation	Cornell University, Ithaca, NY
	Zhang	Ming-Jian	6	Energy Research	Peking University, China
18-3					
	Baltrusaitis	Jonas	3	Material Science	Lehigh University
	Bock	David	15	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Eusterhues	Karin	9	Earth Science	Friedrich-Schiller-University, Jena, Germany
	Gao	Yan	6	Proprietary	General Electrics, Niskayuna, NY
	Hernandez	Victoria	6	Education	William Floyd High School, Mastic Beach, NY
	Holt	Troy	6	Geoscience	Stony Brook University, Stony Brook, NY
	Jain	Himanshu	9	Material Science	Lehigh University
	Keiluweit	Marco	9	Earth Science	University of Massachusetts, Amherst, MA
	Krick	Brandon	3	Material Science	Lehigh University
	Miller	Lisa	12	Bioscience	BNL
	Nicholas	Sarah	9	Planetary Science	Stony Brook University, Stony Brook, NY
	Schlesinger	Danielle	12	Environmental Science	Princeton University, Princeton, NJ
	Wang	Feng	15	Energy Research	BNL
	Woll	Arthur	15	Instrumentation	Cornell University, Ithaca, NY
18-2					
	Bock	David	9	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Chou	Kang Wei	9	Material Science	Henkel Corporation, Duesseldorf, Germany
	Hernandez	Victoria	6	Education	William Floyd High School, Mastic Beach, NY
	Holt	Troy	6	Geoscience	Stony Brook University, Stony Brook, NY
	Lavely	Eugene	15	Material Science	BAE Systems, Burlington, MA
	Legett	Carey	9	Planetary Science	Stony Brook University, Stony Brook, NY
	Miller	Lisa	12	Bioscience	BNL
	Nicholas	Sarah	9	Bioscience	Stony Brook University, Stony Brook, NY
	Woll	Arthur	15	Instrumentation	Cornell University, Ithaca, NY
	Zhang	Ming-Jian	9	Energy Research	Peking University
18-1					
	Avellan	Astrid	12	Earth Science	Carnegie Mellon University, Pittsburgh, PA
	Bock	David	15	Energy Research	Stony Brook University, Stony Brook, NY
	Chou	Kang Wei	15	Material Science	Henkel Corporation, Duesseldorf, Germany
	Hernandez	Victoria	6	Education	William Floyd High School, Mastic Beach, NY

	Jain	Himanshu	12	Material Science	Lehigh University
	Miller	Lisa	18	Bioscience	BNL
	Schlesinger	Danielle	12	Environmental Science	Princeton University, Princeton, NJ
	Sharma	Aakriti	15	Earth Science	North Carolina State University, Raleigh, NC
	Wang	Feng	9	Energy Research	BNL
17-3					
	Avellan	Astrid	12	Earth Science	Carnegie Mellon University, Pittsburgh, PA
	Elbakhshwan	Mohamed	9	Nuclear Science	BNL
	Hossain	Anwar	6	Material Science	BNL
	Keiluweit	Marco	9	Earth Science	University of Massachusetts, Amherst, MA
	Legett	Carey	12	Planetary Science	Stony Brook University, Stony Brook, NY
	Schoonen	Martin	6	Environmental Science	BNL
	Sharma	Aakriti	9	Earth Science	North Carolina State University, Raleigh, NC
	Sprouster	David	9	Nuclear Science	BNL
	Takeuchi	Esther	15	Energy Research	Stony Brook University, Stony Brook, NY
	Vasudevamurthy	Gokul	9	Nuclear Science	General Atomics Corporation, San Diego, CA
17-2					
	Bock	David	15	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Bohle	Scott	9	Bioscience	McGill University, Montreal, Canada
	Chen-Wiegart	Yu-chen	9	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Liao	Hui-Ling	9	Environmental Science	University of Florida, Gainesville, FL
	Mozer	Bob	9	Education	William Floyd High School, Mastic Beach, NY
	Sharma	Aakriti	12	Earth Science	North Carolina State University, Raleigh, NC
	Williams	Garth	15	Instrumentation	BNL
17-1					
	Acerbo	Alvin	6	Geoscience	BNL
	Elbakhshwan	Mohamed	9	Nuclear Science	BNL
	Jain	Himanshu	9	Material Science	Lehigh University
	Moffet	Ryan	9	Environmental Science	University of the Pacific, Stockton, CA
	Hossain	Anwar	9	Material Science	BNL
	Tutolo	Benjamin	9	Geoscience	University of Oxford, United Kingdom
	Gray-Georges	Monica	6	Environmental Science	Lincoln University, Lincoln University, PA
	Park	Alissa	9	Environmental Science	Columbia University, New York, NY
	Galloway	Joshua	6	Energy Research	City College of New York, New York, NY
	Kaczmarek	Janet	6	Education	Sayville High School, Sayville, NY
	LeVaillant	Margaux	15	Instrumentation	CSIRO, Melbourne, Australia
	Unrine	Jason	9	Earth Science	University of Kentucky, Lexington, KY
	Wang	Feng	12	Energy Research	BNL
16-3					
	Acerbo	Alvin	9	Geoscience	BNL
	Bohle	Scott	6	Bioscience	McGill University, Montreal, Canada
	Chen-Wiegart	Karen	6	Energy Research	BNL
	Gallaway	Joshua	6	Energy Research	City College of New York, New York, NY
	Gill	Simerjeet	9	Nuclear Science	BNL
	Miller	Lisa	6	Bioscience	BNL
	Petrash	Stan	6	Material Science	Henkel Corporation

	Pellicione	Christopher	9	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Salditt	Tim	12	Instrumentation	Georg-August-University, Goettingen, Germany
	Tappero	Ryan	9	Education	BNL
	Thieme	Juergen	9	Planetary Science	BNL
16-2					
	Acerbo	Alvin	6	Geoscience	BNL
	Ecker	Lynn	12	Nuclear Science	BNL
	Miller	Lisa	9	Bioscience	BNL
	Moffet	Ryan	9	Environmental Science	University of the Pacific, Stockton, CA
	Myneni	Satish	9	Environmental Science	Princeton University, Princeton, NJ
	Punshon	Tracy	9	Earth Science	Dartmouth College, Hanover, NH
	Tchoubar	Oleg	12	Instrumentation	BNL
	Thieme	Juergen	12	Planetary Science	BNL
	Tyson	Trevor	9	Material Science	New Jersey Institute of Technology, Newark, NJ
	Unrine	Jason	9	Earth Science	University of Kentucky, Lexington, KY
16-1					
	Blaby	Crysten	6	Bioscience	BNL
	Centeno	Silvia	9	Cultural Heritage	Metropolitan Museum of Art, New York, NY
	Chen-Wiegart	Karen	9	Material Science	BNL
	Chen-Wiegart	Karen	9	Energy Research	BNL
	Chorover	Jon	9	Environmental Science	University of Arizona, Tuscon, AZ
	Gallaway	Joshua	9	Energy Research	City College of New York, New York, NY
	Hesterberg	Dean	9	Earth Science	North Carolina State University, Raleigh, NC
	Jain	Himanshu	9	Material Science	Lehigh University
	Takeuchi	Esther	6	Energy Research	Stony Brook University, Stony Brook, NY, and BNL
	Tchoubar	Oleg	9	Instrumentation	BNL
	Woloschak	Gayle	9	Bioscience	Northwestern University, Chicago, IL
15-3					
	Chorover	Jon	9	Environmental Science	University of Arizona, Tuscon, AZ
	Hesterberg	Dean	9	Earth Science	North Carolina State University, Raleigh, NC
	Jain	Himanshu	9	Material Science	Lehigh University
	Myneni	Satish	9	Environmental Science	Princeton University, Princeton, NJ
	Schoonen	Martin	9	Environmental Science	BNL
15-2					
	Chen-Wiegart	Karen	18	Material Science	BNL
	Frenkel	Anatoly	12	Material Science	Yeshiva University, New York, NY
	Salditt	Tim	18	Instrumentation	Georg-August-University, Goettingen, Germany
	Schoonen	Martin	9	Environmental Science	BNL

Table SI-2: User and SRX staff publications. Those using beamtime without co-authorship of SRX staff are marked (**), beamline staff publications using other beamlines or facilities are marked (*).

Year	Publication	Imp.Fac.
2019		
	Huie, M.M., Bock, D.C., Bruck, A.M., Tallman, K.R., Housel, L.M., Wang, L., Thieme, J., Takeuchi, K.J., Takeuchi, E.S., Marschilok, A.C.: Isothermal Microcalorimetry: Insight into the Impact of Crystallite Size and Agglomeration on the Lithiation of Magnetite, Fe3O4. *ACS Applied Materials & Interfaces*, *11*, 7074–7086. https://doi.org/10.1021/acsami.8b20636	8.1
	Zheng, J., Zhao, Q., Liu, X., Tang, T., Bock, D.C., Bruck, A.M., Tallman, K.R., Housel, L.M., Kiss, A.M., Marschilok, A.C., Takeuchi, E.S., Takeuchi, K.J., Archer, L.A.: Nonplanar Electrode Architectures for Ultrahigh Areal Capacity Batteries. ACS Energy Letters, 4(1), 271–275. Rapid Communication. https://doi.org/10.1021/acsenergylett.8b02131	12.3
	Rod, K. A., Nguyen, M.-T., Elbakhshwan, M., Gills, S., Kutchko, B., Varga, T., Mckinney, A.M., Roosendaal, T.J., Childers, M.I., Zhao, C., Chen-Wiegart, Y.C.K., Thieme, J., Koech, P.K., Um, W., Chun, J., Rousseau, R., Glezakou, V.A., Fernandez, C. A.: Insights into the physical and chemical properties of a cement-polymer composite developed for geothermal wellbore applications. *Cement and Concrete Composites*, *97*, 279–287. https://doi.org/10.1016/j.cemconcomp.2018.12.022	5.4
	Li, J., Tappero, R.V., Acerbo, A.S., Yan, H., Chu, Y., Lowry, G.V., Unrine, J. M.: Effect of CeO2 nanomaterial surface functional groups on tissue and subcellular distribution of Ce in tomato (Solanum lycopersicum) . Environmental Science: Nano, 6(1), 273–285. https://doi.org/10.1039/c8en01287c	6.1
2018		
**	Allwood, A.C., Rosing, M.T., Flannery, D.T., Hurowitz, J.A., Heirwegh, C.M.: Reassessing evidence of life in 3,700-million-year-old rocks of Greenland. *Nature* 563, 241–244 https://doi.org/10.1038/s41586-018-0610-4	41.6
**	Wang, L., Bock, D.C., Li, J., Stach, E.A., Marschilok, A.C., Takeuchi, K.J., Takeuchi, E.S.: Synthesis and Characterization of CuFe2O4 Nano/Submicron Wire-Carbon Nanotube Composites as Binder-free Anodes for Li-Ion Batteries. *ACS Applied Materials and Interfaces*, *10*(10), 8770–8785. https://doi.org/10.1021/acsami.8b00244	8.1
**	Hammond, C.M., Root, R.A., Maier, R.M., Chorover, J.: Mechanisms of Arsenic Sequestration by Prosopis juliflora during the Phytostabilization of Metalliferous Mine Tailings. Environmental Science and Technology, 52(3), 1156–1164. https://doi.org/10.1021/acs.est.7b04363	6.7
	Zhang, M.-J., Teng, G., Chen-Wiegart, Y.C.K., Duan, Y., Ko, J.Y.P., Zheng, J., Thieme, J., Dooryhee, E., Chen, Z., Bai, J., Amine, K.,Pan, F., Wang, F.: Cationic Ordering Coupled to Reconstruction of Basic Building Units during Synthesis of High-Ni Layered Oxides. Journal of the American Chemical Society, 140(39), 12484–12492. https://doi.org/10.1021/jacs.8b06150	14.4
	Gallaway, J.W., Yadav, G.G., Turney, D.E., Nyce, M., Huang, J., Chen-Wiegart, Y.C.K., Williams, G., Thieme, J., Okasinski, J.S., Wei, X., Banerjee, S.: An Operando Study of the Initial Discharge of Bi and Bi/Cu Modified MnO 2. *Journal of The Electrochemical Society*, *165*(13), A2935–A2947. https://doi.org/10.1149/2.0221813jes	3.7
	Jones, M.E., Nico, P.S., Ying, S., Regier, T., Thieme, J., Keiluweit, M.: Manganese-Driven Carbon Oxidation at Oxic-Anoxic Interfaces. *Environmental Science and Technology*, *52*(21), 12349–12357. https://doi.org/10.1021/acs.est.8b03791	6.7

	Thieme, J., Hurowitz, J., Schoonen, M., Farley, K., Sherman, S., & Hill, J.: Elemental Composition of Analogs to Mars Return Samples Studied with X-Ray Fluorescence Imaging at NSLS-II. *Microscopy and Microanalysis* 24, 498-499. https://doi.org/10.1017/s1431927618014721	
	Vanderschee, C.R., Kuter, D., Bolt, A.M., Lo, F., Feng, R., Thieme, J., Chen-Wiegart, Y.C.K., Williams, G., Mann, K.K., Bohle, D.S.: Accumulation of persistent tungsten in bone as in situ generated polytungstate. *Nature Communications Chemistry*, *1*(1), 1–6. https://doi.org/10.1038/s42004-017-0007-6	
	Chubar, O., Kitegi, C., Chen-Wiegart, Y.C.K., Hidas, D., Hidaka, Y., Tanabe, T., Williams, G., Thieme, J., Caswell, T.,Rakitin, M., Wiegart, L., Fluerasu, A., Yang, L., Chodankar, S., Zhernenkov, M.: Spectrum-Based Alignment of In-Vacuum Undulators in a Low-Emittance Storage Ring. Synchrotron Radiation News, 31(3), 4–8. https://doi.org/10.1080/08940886.2018.1460173	
*	Prietzel, J., Mueller, S., Koegel-Knabner, I., Thieme, J., Jaye, C., Fischer, D.: Comparison of soil organic carbon speciation using C NEXAFS and CPMAS 13C NMR spectroscopy, *Science of the Total Environment*, 628-629, 906-918. https://doi.org/10.1016/j.scitotenv.2018.02.121	4.6
2017		
	Chen-Wiegart, Y.C.K., Catalano, J., Williams, G.J., Murphy, A., Yao, Y., Zumbulyadis, N., Centeno, S.A., Dybowski, C., Thieme, J.: Elemental and Molecular Segregation in Oil Paintings due to Lead Soap Degradation. *Scientific Reports*, 7:11665, 1-9. https://doi.org/10.1038/s41598-017-11525-1	4.1
	Sun, K., Zhao, C., Lin, C.H., Stavitski, E., Williams, G.J., Bai, J., Dooryhee, E., Attenkofer, K., Thieme, J., Chen-Wiegart, Y.C.K., Gan, H.: Operando Multi-modal Synchrotron Investigation for Structural and Chemical Evolution of Cupric Sulfide (CuS) Additive in Li-S battery. *Scientific Reports*, 7:12976, 1–10. https://doi.org/10.1038/s41598-017-12738-0	4.1
	Zhao, C., Wada, T., De Andrade, V., Williams, G.J., Gelb, J., Li, L.,Thieme, J., Kato, H., Chen-Wiegart, Y.C.K.: Three-dimensional morphological and chemical evolution of Nanoporous stainless steel by liquid metal dealloying. *ACS Applied Materials and Interfaces*, *9*(39), 34172–34184. https://doi.org/10.1021/acsami.7b04659	8.1
	Chubar, O., Caswell, T., Chen-Wiegart, Y.C.K., Fluerasu, A., Hidaka, Y., Hidas, D., Kitegi, C., Rakitin, M., Tanabe, T., Thieme, J., Wiegart, L., Williams, G.: Analysis and Correction of In-vacuum Undulator Misalignment Effects in a Storage Ring Synchrotron Radiation Source, Proceedings of IPAC2017, p. 1663-1665, sponsored by IPAC2017 (2017).	
	Palomino, R.M., Stavitski, E., Waluyo, I., Chen-Wiegart, Y.C.K., Abeykoon, M., Sadowski, J.T., Rodriguez, J.A., Frenkel, A.I., Senanayake, S.D.: New In-Situ and Operando Facilities for Catalysis Science at NSLS-II: The Deployment of Real-Time, Chemical, and Structure-Sensitive X-ray Probes. Synchrotron Radiation News, 30(2), 30–37. https://doi.org/10.1080/08940886.2017.1289805	
**	Yadav, G.G., Gallaway, J.W., Turney, D.E., Nyce, M., Huang, J., Wei, X., Banerjee, S.: Regenerable Cu-intercalated MnO2 layered cathode for highly cyclable energy dense batteries. *Nature Communications,* 8:14424, 1-9. https://doi.org/10.1038/ncomms14424	12.4
	Thieme, J., Hurowitz, J., Dooryhee, E., Fogelqvist, E., Gregerson, J., Schoonen, M., Farley, K., Sherman, S.: Elemental Composition of Analogs to Samples Returned from Mars Using X-Ray Fluorescence Imaging at the National Synchrotron Light Source II at Brookhaven National Laboratory. 48th Lunar and Planetary Science Conference, Vol 1964, id.2265, sponsored by LPI Contribution.	
*	Amaya, A., Pathak, H., Modak, V., Laksmono, H., Loh, N.D., Sellberg, J., Sierra, R., McQueen, T., Williams, G.J., Messerschmidt, M., Boutet, S., Bogan, M.J., Nilsson, A., Stan, C.A., Wyslouzil, B.E.: How Cubic Can Ice Be?, J. Phys. Chem. Letts., 8(14), 3216-3222	8.7

*	Hosseinizadeh, A., Mashayekhi, G., Copperman, J., Schwander, P., Dashti, A., Sepehr, R., Fung, R., Schmidt, M., Yoon, C.H., Hogue, B.G., Williams, G.J., Aquila, A., Ourmazd, A.: Conformational Landscape of a Virus by Single-particle X-ray Scattering, *Nature Methods*, 14, 877-881	26.9
*	Werner, F., Mueller, C.W., Thieme, J., Gianoncelli, A., Rivard, C., Hoeschen, C., Prietzel, J.: Micro-scale heterogeneity of soil phosphorus depends on soil substrate and depth. Scientific Reports, 7(1), 1–9. https://doi.org/10.1038/s41598-017-03537-8	4.1
*	Hesterberg, D., McNulty, I., & Thieme, J. (2017). Speciation of Soil Phosphorus Assessed by XANES Spectroscopy at Different Spatial Scales. Journal of Environmental Quality, 46(6), 1190. https://doi.org/10.2134/jeq2016.11.0431	2.4
2016		
	Chen-Wiegart, Y.C.K., Williams, G., Zhao, C., Jiang, H., Li, L., Demkowicz, M., Seita, M., Short, M., Ferry, S., Wada, T., Kato, H., Chou, K.W., Petrash, S., Catalano, J., Yao, Y., Murphy, A., Zumbuyadis, N., Centeno, S.A., Dybowski, C., Thieme, J.: Early science commissioning results of the sub-micron resolution X-ray spectroscopy beamline (SRX) in the field of materials science and engineering. *AIP Conference Proceedings*, *1764*. https://doi.org/10.1063/1.4961138	
	Jiang, H., Chou, K.W., Petrash, S., Williams, G., Thieme, J., Nykypanchuk, D., Li, L., Muto, A., Chen-Wiegart, Y.C.K.: Environmentally induced chemical and morphological heterogeneity of zinc oxide thin films. *Applied Physics Letters*, *109*(9). https://doi.org/10.1063/1.4962203	3.5
	Chubar, O., Chu, Y.S., Huang, X., Kalbfleisch, S., Yan, H., Shaftan, T., Wang, G., Cai, Y.Q., Suvorov, A., Fluearasu, A., Wiegart, L., Chen-Wiegart, Y.C.K., Thieme, J., Williams, G., Idir, M., Tanabe, T., Zschack, P., Shen, Q.: Initial performances of first undulator-based hard x-ray beamlines of NSLS-II compared to simulations. *AIP Conference Proceedings*, *1741*. https://doi.org/10.1063/1.4952874	
*	Wang, J., Chen-Wiegart, Y.C.K., Eng, C., Shen, Q., Wang, J.: Visualization of Anisotropic-isotropic Phase Transformation Dynamics in Battery Electrode Particles, *Nature Communications*, 7, 12372	12.4
*	Chen-Wiegart, Y.C.K., Kennouche, K., Cronin, J.S., Barnett, S., Wang, J.: Effect of Ni Content on the Morphological Evolution of Ni-YSZ Solid Oxide Fuel Cell Electrodes, Appl. Phys. Lett., 108, 083903	3.5
*	Cho, H., Chen-Wiegart, Y.C.K., Dunand, D.: Finite Element Analysis of Mechanical Stability of Coarsened Nanoporous Gold, *Scripta Mater.*, **115**, 96-99	4.2
*	Kennouche, D., Chen-Wiegart, Y.C.K., Riscoe, C., Wang, J., Barnett, S.: Combined Electrochemical and X-ray Tomography Study of the High Temperature Evolution of Nickel – Yttria Stabilized Zirconia Solid Oxide Fuel Cell Anodes, *J. Power Sources*, 307, 604-612	6.9
*	Szlachetko, J., Hoszowska, J., Dousse, J., Nachtegaal, M., Blachucki, W., Kayser, Y., Sa, J., Messerschmidt, M., Williams, G., David, C., Smolentsev, G., van Bokhoven, J.A., Patterson, B.D., Penfold, T.J., Knopp, G., Pajek, M., Abela, R., Milne, C.J.: Establishing Nonlinearity Thresholds with Ultraintense X-ray Pulses, *Scientific Reports*, 6, 33292	4.1
	Lin, M., Xin, H., Chu, Y., Yan, H., Tappero, R., Thieme, J., Lee, W.-K., Biersach, D., Smart, J., Jones, K., Titarenko, V.: Towards a portable open-source tomography toolbox: Containerizing tomography software with docker. AIP Conference Proceedings, 1764. https://doi.org/10.1063/1.4961142	
2015		
*	Nave, M., Chen-Wiegart, Y.C.K., Wang, J., Kornev, K.: Precipitation and Surface Adsorption of Metal Complexes During Electropolishing. Theory and Characterization with X-ray Nanotomography and Surface Tension Isotherms. *Phys. Chem. Chem. Phys.*, 17, 23121-23131	3.9

*	Li, L., Chen-Wiegart, Y.C.K., Wang, J., Gao, P., Ding, Q., Yu, Y., Wang, F., Cabana, J., Wang, J., Jin, S.: Visualization of Electrochemically Driven Solid-state Phase Transformations Using Operando Hard X-ray Spectro-imaging, *Nature Communications*, 6, 6883	12.4
*	Wang, J., Eng, C., Chen-Wiegart, Y.C.K., Wang, J.: Probing Three-dimensional Sodiation–desodiation Equilibrium in Sodium-ion Batteries by in situ Hard X-ray Nanotomography, *Nature Communications*, 6, 7496	12.4
	Stach, E.A., Li, Y., Zhao, S., Gamalski, A., Zakharov, D., Tappero, R., Chen-Weigart, Y.C.K., Thieme, J., Jung, U., Elsen, A., Wu, Q., Orlov, A., Chen, J., Nuzzo, R.G., Frenkel, A.: Characterizing Working Catalysts with Correlated Electron and Photon Probes. *Microscopy and Microanalysis*, 21(S3), 563–564.	
2014		
	Gregoire, P., Engelbrektson, A., Hubbard, C.G., Metlagel, Z., Csencsits, R., Auer, M., Conrad, M.E., Thieme, J., Northrup, P., Coates, J.D.: Control of sulfidogenesis through bio-oxidation of H2S coupled to (per)chlorate reduction. Environmental Microbiology Reports. https://doi.org/10.1111/1758-2229.12156	2.9
*	Abel, S., Nehls, T., Mekiffer, B., Mathes, M., Thieme, J., Wessolek, G.: Pools of sulfur in urban rubble soils. *Journal of Soils and Sediments*, 15(3), 532–540. https://doi.org/10.1007/s11368-014-1014-1	2.6
*	De Andrade, V., Ganne, J., Dubacq, B., Ryan, C.G., Bourdelle, F., Plunder, A., Falkenberg, G., Thieme, J.: Retrieving past geodynamic events by unlocking rock archives with µ-XRF and µ-spectroscopy. *Journal of Physics: Conference Series*, *499*(1). https://doi.org/10.1088/1742-6596/499/1/012012	
2013		
*	Michot, L., Bihannic, I., Thomas, F., Lartiges, B., Waldvogel, Y., Cailles, C., Thieme, J., Funari, S., Levitz, P.: Coagulation of Na-Montmorillonite by Inorganic Cations at Neutral pH. A Combined Transmission X-ray Microscopy, Small Angle and Wide Angle X-ray Scattering Study, *Langmuir*, 29, 3500-3510.	3.8
*	Thieme, J., Kilcoyne, D., Tyliszczak, T., Haselwandter, K.: Spatially Resolved NEXAFS Spectroscopy of Siderophores in Biological Matrices, J Phys.: Conf. Ser., 463, 012037	
*	Liu, X., Eusterhues, K., Thieme, J., Ciobota, V., Hoeschen, C., Mueller, C., Kuesel, K., Koegel-Knabner, I., Roesch, P., Popp, J., Totsche, K.-U.: STXM and NanoSIMS Investigations on EPS Fractions Before and After Adsorption to Goethite, Environ. Sci. Tech., 47, 3158-3166	6.1
2012		
*	Rennert, T., Totsche, K.-U., Heister, K., Kersten, M., Thieme, J.: Advanced Spectroscopic, Microscopic, and Tomographic Characterization Techniques to Study Biogeochemical Interfaces in Soil, J. Soils Sediments, 12, 3-23	2.6
*	Sedlmair, J., Gleber, S., Wirick, S., Guttmann, P., Thieme, J.: Interaction Between Carbon Nanotubes and Soil Colloids Studied with X-ray Spectromicroscopy, Chem. Geol., 329, 32ff	3.6
2011		
*	Prietzel, J., Koegel-Knabner, I., Thieme, J., Paterson, D., McNulty, I.: Microheterogeneity of Element Distribution and Sulfur Speciation in an Organic Surface Horizon of a Forested Histosol as Revealed by Synchrotron-based X-ray Spectromicroscopy, Org. Geoch., 42(11), 1308-1314	2.8
	De Andrade, V., Thieme, J., Northrup, P., Yao, Y., Lanzirotti, A., Eng, P., Shen, Q.: The sub-micron resolution X-ray spectroscopy beamline at NSLS-II. *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, *649*(1), 46–48. https://doi.org/10.1016/j.nima.2010.11.154	1.3
	De Andrade, V., Thieme, J., Chubar, O., Idir, M.: Simulation and optimization of the NSLS-II SRX beamline combining ray- tracing and wavefront propagation, Proc. SPIE 8141, Advances in Computational Methods for X-Ray Optics II, 81410L; doi: 10.1117/12.894954	