

NSLS-II Beamline Report for SAC Review of Beamlines

Beamline: *In situ and Operando Soft X-ray Spectroscopy (IOS, 23-ID-2)*

Report Date: September 10, 2018

Introduction

IOS (23-ID-2) is a soft X-ray beamline on the cell 23 straight section, sharing EPU49 sources with the CSX (23-ID-1) beamline. The focus at IOS is *in situ* and *operando* chemistry using soft X-ray spectroscopic techniques, such as ambient pressure X-ray photoelectron spectroscopy (AP-XPS) and X-ray absorption spectroscopy (XAS), with a scientific focus on studying energy materials and processes such as heterogeneous catalysis, fuel cells, photovoltaics, and batteries, in close-to-realistic working conditions. This scientific and technical focus is aligned with the NSLS-II science priority area of “Operando Chemistry and Structural Science” outlined in the NSLS-II Strategic Plan document.

23-ID-2, initially called CSX-2, was funded as a part of the initial NSLS-II project beamlines. The construction of the 23-ID beamlines was completed in 2014. The first light on the 23-ID-2 branch was achieved on March 23, 2015. The beamline and endstation were commissioned in cycles 2015-2 and 2015-3, respectively. The beamline was approved for general user (GU) operation on November 10, 2015, and GU experiments started in January 2016 (cycle 2016-1). The name change from CSX-2 to IOS was approved in March 2018 to more accurately represent the current techniques and science performed at the beamline.

Beamline Overview

The beamline provides soft X-ray photons with an energy range of 250 to 2000 eV, photon flux of up to 3×10^{13} photons/s, resolving power of $10^4 E/\Delta E$, and a focused spot size of $70 \mu\text{m}$ (h) \times $15 \mu\text{m}$ (v). A layout of the beamline is shown in Figure 1, showing the important optical components including the two EPUs, toroidal horizontally focusing mirrors, variable line spacing plane grating monochromator (VLS-PGM), vertical exit slit, and an elliptical vertically focusing mirror. The EPUs can be operated in one of two modes: (1) straight mode with the canting magnet out, where one X-ray beam is propagated down either CSX or IOS, with one beamline operating at a time, or (2) canted mode with the canting magnet in place, where two X-ray beams are produced, one for each branch. In theory, the two 23-ID beamlines CSX and IOS can be operated simultaneously in the canted mode, but due to interference issues (see details in Appendix A), CSX and IOS split the operating schedule on 50-50 basis.

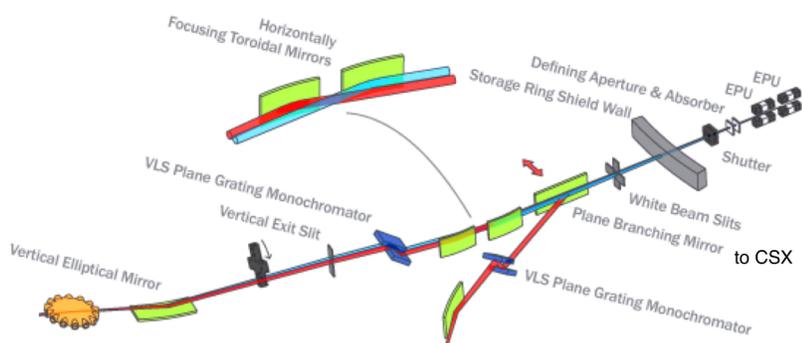


Figure 1. Schematics of the beamline layout

Two endstations are available at IOS: ambient pressure photoelectron spectroscopy (APPEs), and in situ and operando X-ray absorption spectroscopy (IO-XAS). The schematic for each endstation is shown in Figure 2.

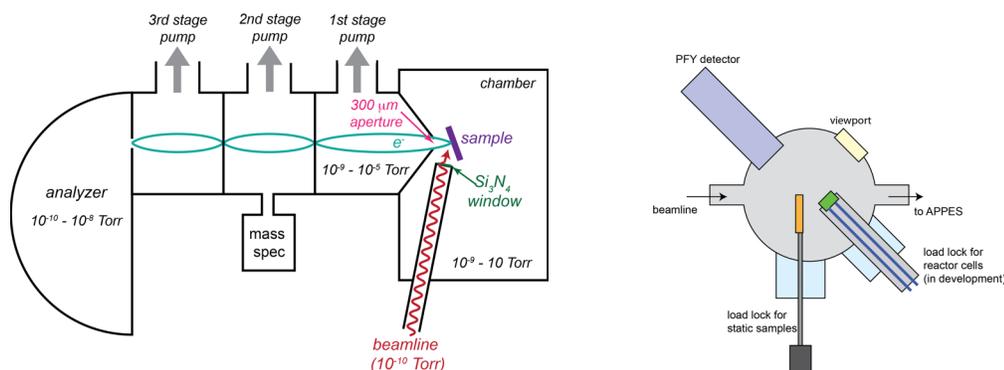


Figure 2. Schematics of the APPEs (left) and IO-XAS (right) endstations

The APPEs endstation is available for general users. It allows AP-XPS and AP-XAS (in electron yield mode) experiments in elevated gas pressures. Through the use of a SPECS Phoibos 150 NAP analyzer with three differential pumping stages and a 300 μm aperture between the main chamber and the first differential pumping stage, the analyzer remains in high vacuum while the pressure in the main chamber can be increased up to 10 Torr. The beamline's UHV environment is separated from the main chamber by a 100 nm-thick Si_3N_4 window. A mass spectrometer is available in the second pumping stage of the analyzer, so that the composition of the gases near the surface of the sample can be analyzed to obtain reactivity information. The gas handling consists of gas sources in lecture bottles, a gas manifold, and manually-operated variable leak valves. Samples are mounted on a Thermionics sample holder and transfer system through a load-lock. Sample heating can be done up to 900°C in UHV and 500-600°C in ambient pressures, depending on the type of gas and pressure. Available surface preparation tools include a sputter ion gun and a 4-pocket e-beam evaporator (both from SPECS). At the writing of this report, the AP-XPS capability has been down since May 2018 due to problems with the analyzer, which had to be shipped to Germany for repairs.

The IO-XAS endstation is currently available for general users for *ex situ* XAS measurements of UHV compatible samples in total electron yield (TEY) and partial fluorescence yield (PFY) detection modes. TEY is done through drain current measurements while PFY uses an energy discriminating silicon drift detector (Vortex EM). The sample holder is capable of holding up to 8 samples and data acquisition for multiple edges across multiple samples can be automated through Bluesky. A glove bag may be used for air-free sample loading. A new sample holder capable of applying an electrochemical potential on a sample was recently developed, and it is available for science commissioning. The *in situ* capabilities are in development (details are in the "Vision for the next five years" section).

The largest scientific community at IOS performs heterogeneous catalysis research using both AP-XPS and XAS (~65% of proposals). AP-XPS, in particular, is an extremely powerful technique in studying heterogeneous catalytic systems. In addition to the strengths of XPS, such as surface sensitivity, elemental specificity, sensitivity to the chemical and physical environments of the probed atom, and quantification and depth profiling capabilities, AP-XPS also enables experiments to be performed at elevated pressures, which are closer to the working environments of catalysts. This allows researchers to bridge the so-called "pressure gap" between conventional UHV experiments and real industrial processes. Materials science research, mainly for materials with potential applications in fuel cells and

photovoltaics, represent ~25% of proposals submitted to IOS. The battery community represents a smaller (~10%) but growing group of users at IOS, especially with XAS.

Data acquisition on the IO-XAS endstation is done through Bluesky, the standard NSLS-II software. This allows the use of Python scripts to automate measurements and control the beamline and endstation components such as motors, detectors, shutters, and gate valves. Data acquisition on the APPES endstation uses the SpecsLab Prodigy software run on a Windows machine. We plan to integrate the AP-XPS analyzer into EPICS to allow the use of scripts as well as enable PEY-XAS measurements using the analyzer synchronously with the photon energy scan, which is currently not possible. Data analysis is performed by each individual user group using their preferred software. User labs available for IOS users include 1LL04 (dry lab), 1LL07 (wet lab), and 3LL09 (wet lab with an Ar glove box).

The beamline staff at IOS are the following:

1. Iradwikanari Waluyo (Associate Chemist, Lead Beamline Scientist), expertise: AP-XPS, XAS, and IRRAS in surface science and heterogeneous catalysis, XAS of water and aqueous solutions
2. Adrian Hunt (Science Associate in the SXSS program, matrixed at 75% as IOS beamline scientist), expertise: XAS and XES/RIXS in materials science and condensed matter physics

Productivity and Impact

A. Science examples from IOS

1. *In situ* surface characterization of Pt-Cu single atom alloy model system with AP-XPS (internal staff research, published in *J. Phys Chem. C*, 122, 4488(2018))

Pt-Cu single atom alloy (SAA) catalysts, in which Pt atoms at low loadings are atomically dispersed on Cu support, are recently found to be promising hydrogenation catalysts with a significantly reduced cost due to the minimized use of Pt. Its activity in hydrogen dissociation, which is the rate-limiting step in hydrogenation reactions, was found to match that of pure Pt, and it was proposed to be resistant to poisoning by CO. The model system of this catalyst has been extensively studied under UHV conditions with low temperature STM and temperature-programmed desorption experiments, but its surface properties under reaction conditions had not been explored. At IOS, AP-XPS was used to study the interaction between the Pt/Cu(111) SAA model system with ambient pressure of CO. Taking advantage of the surface sensitivity of the technique as well as high energy resolution of the beamline to distinguish different chemical and physical states, we used the Pt 4f core level to monitor the evolution of the Pt atoms in different experimental conditions. We found that the surface Pt atoms are not stable in UHV as they diffuse into the subsurface and deeper into the bulk of Cu upon heating above 400 K. However, the presence of CO at ambient pressures stabilize Pt atoms and prevent the diffusion of surface Pt atoms at up to 500 K. In a case where surface Pt has been lost due to subsurface/bulk diffusion after heating in UHV, treatment in CO at 500 K can be used to draw out Pt atoms from the subsurface and bulk layers back to the surface, thereby restoring the initial surface composition (Fig. 3). However, this thermal stability in CO comes at the expense of slightly strengthened Pt-CO interaction, likely due a restructuring in the subsurface layer. This work provides fundamental insight on how the SAA behaves in reaction conditions and emphasizes the necessity of studying a catalytic system using *in situ* methods such as AP-XPS.

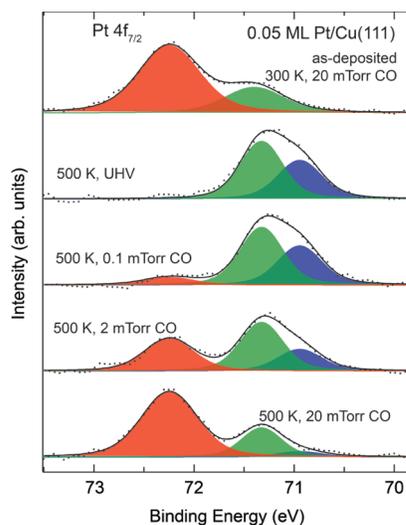


Figure 3. Pt 4f XPS of 0.05 ML Pt/Cu(111) in various experimental conditions.

2. *Surface defect of Pr_{0.1}Ce_{0.9}O_{2-δ} with operando AP-XAS (Yildiz Group, MIT, published in Chem. Mater. 30, 2600 (2018))*

Doped ceria are often studied for their potential application in solid oxide fuel cells (SOFC) and solid oxide electrolysis cells (SOEC). It is, therefore, important to understand their behavior in highly oxidizing environments to mimic the operating conditions of SOFC cathodes or SOEC anodes. Using partial electron yield (PEY) AP-XAS combined with solid state electrochemical methods, the group of Prof. Bilge Yildiz from MIT was able to study changes in the oxidation state of Pr on the surface of Pr_{0.1}Ce_{0.9}O_{2-δ} *in operando*. By applying an electrochemical potential of -0.5 V to 0.5 V to the sample in 200 mTorr of O₂ at 450°C, they were able to achieve an effective O₂ pressure range from 10⁻¹⁵ to 10⁷ atm. Since XAS is highly sensitive to the oxidation state of the metal, they were able to quantify the fraction of Pr³⁺ to Pr⁴⁺ at different effective O₂ pressure (Fig. 4). They discovered that the surface of the Pr-doped ceria contains a higher concentration of the reduced Pr³⁺ species than the bulk at the same effective O₂ pressure. This indicates a lower surface defect formation energy even in highly oxidizing conditions and that the surface defect chemistry cannot be predicted from the bulk model. This research provides a deeper understanding of how the surface of these materials behave under real operating conditions, which potentially aids in the design of better SOFC and SOEC electrodes.

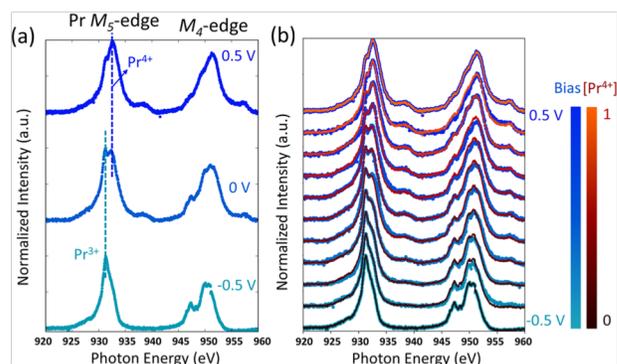


Figure 4. Pr M_{4,5}-edge XAS of Pr_{0.1}Ce_{0.9}O_{2-δ} at different electrochemical potential in 200 mTorr O₂ at 450°C

3. *Water Dissociation and Surface Hydroxyl Stability on Pure and Ni-Modified CoOOH (Koel Group, Princeton, published in J. Phys. Chem. B 122, 810 (2018))*

Metal oxide and oxyhydroxide catalysts are important in oxygen evolution reaction (OER) in alkaline conditions, which is a half reaction in water electrolysis. Cobalt-based oxides and oxyhydroxides, in particular, are demonstrated to have excellent OER activities comparable to the precious metal counterparts. Nickel doping of CoOOH has been proposed to improve its activity. Since the dissociation of water to OH (hydroxyl) species is an important elementary step in OER, Prof. Bruce Koel's group from Princeton used AP-XPS to study pure and Ni-modified CoOOH nanowires in an ambient pressure of water to investigate the dissociation of water and stabilization of the resulting hydroxyl species. Through the observation of adsorbed OH species, they found that both samples readily dissociate water at room temperature, which is attributed to the presence of oxygen vacancies on the surface. In addition, they observed that Ni doping promotes the formation of Co²⁺ at higher temperatures. More importantly, the surface hydroxyl was found to be more thermally stable on the Ni-modified sample as a higher fraction of the OH species remains on the surface above 200°C on the Ni-modified sample compared to on the pure CoOOH sample (Fig. 5), in agreement with

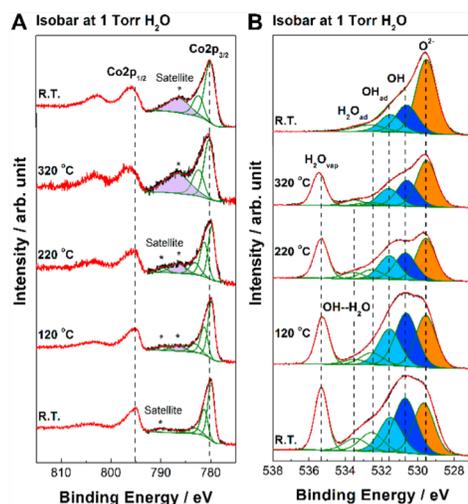


Figure 5. Co 2p (left) and O 1s (right) XPS of Ni-modified CoOOH nanowires in 1 Torr H₂O

results from DFT calculations. The increased stability of surface hydroxyl plays a key part in OER activity, so this study provides insight that contribute to the rational design of OER catalysts.

B. Partner user program

The APPES endstation is available through a partnership with the Interface Science and Catalysis group at the CFN. The endstation was constructed in early 2010's and it was initially operated at NSLS beamline X1A1 in 2013-2014. It was moved to NSLS-II after NSLS was permanently shut down in September 2014. The partner user agreement (PUA) was activated upon the start of GU operation in January 2016. The PUA stipulates that the CFN receive 23% of the available user time for running their user program as well as their own research, in exchange for an upgraded endstation valued at \$800K and some staffing contributions. However, besides the necessary replacements of failing components over the years (e.g. detector, pumps, valves), the endstation has not been upgraded since its first construction. The three-year term of this PUA is ending by the next cycle. A path forward for a revised partnership with CFN is currently under discussion with CFN management, with an objective to establish a true functional partnership that will benefit both facilities and the broad scientific user community

The IO-XAS endstation is available through a partnership with the Catalysis: Reactivity and Structure group in the BNL Chemistry department. The PU contributes the Vortex detector, manipulator, and *in situ* cells (developed by the Advanced Light Source) for 8% of the available user time. Since the *in situ* cells are not available for GU yet, the PUA has not been activated.

C. Beamline usage statistics

Table 1 shows the number of submitted and allocated proposals, subscription rate, and the number of users every cycle since 2015-3. Fig. 6 shows the graph of submitted and allocated proposals. Cycle 2015-3 was technical commissioning, so no proposals were allocated. Fig. 7 shows the beam time usage per cycle (defined as user-available time = GU+PU+RA+BAG+BDT). IOS currently does not accept RA (rapid access) or BAG (block allocation group) proposals. Table 2 shows the number of unique users per calendar year.

Cycle	Proposals Submitted	Proposals Allocated	Subscription Rate	Users
2015-3	8	0	0.0	40
2016-1	22	9	2.44	72
2016-2	20	11	1.82	80
2016-3	19	9	2.11	59
2017-1	19	10	1.90	68
2017-2	24	9	2.67	99
2017-3	32	15	2.13	72
2018-1	43	13	3.31	62
2018-2	48	16	3.00	24

Table 1. Proposals, subscription rate, and users per cycle

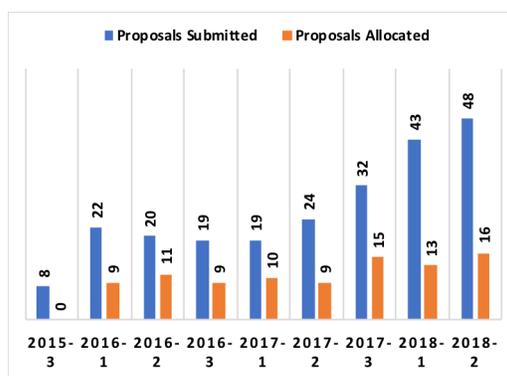


Figure 6. Number of proposals submitted and allocated

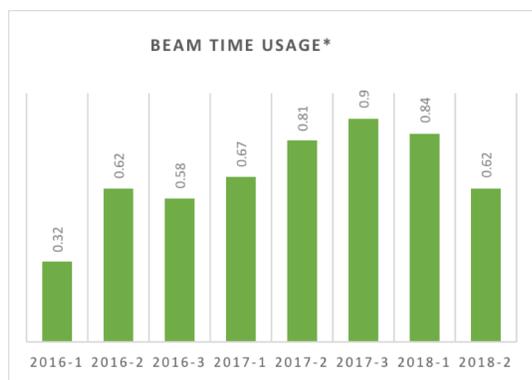


Figure 7. Beam time usage per cycle

CY	Unique users
2015	5
2016	67
2017	90
2018	46

Table 2. Unique users per calendar year

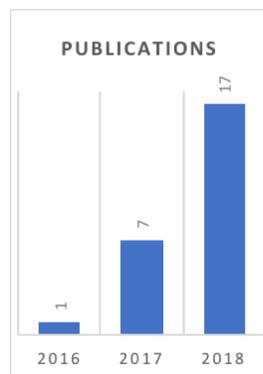


Figure 8. Publications per CY

On average, AP-XPS experiments account for ~75% of beam time. Please note that although 16 proposals were allocated time in 2018-2, the number of users and beam time usage that cycle was lower than in the previous cycle because the AP-XPS analyzer was not operational, so AP-XPS experiments were cancelled. A significant amount of time during 2018-2 cycle was spent on troubleshooting the analyzer. A complete list of users is available in Appendix B.

D. Publications

The number of publications for each calendar year is shown in Fig. 8. A complete list of publications is available in Appendix C.

Vision for Next Five Years

While heterogeneous catalysis remains the largest user community at IOS, there is also growing interest from the materials science and battery communities. We would like to continue fostering the growth of these communities in the next 5 years, but we face a challenge as the available user time is reduced due to the split schedule between CSX and IOS, necessitated by the interference issues described in Appendix A. This is reflected from the higher subscription rate starting in 2018-1 cycle as each beamline essentially operates 50% of the time. A working group was formed to develop a plan to address these issues. We proposed increasing the canting angle from 0.16 to 2 mrad, which will certainly solve the interference issues. This plan requires commitment in terms of cost and some down time for both beamlines. Hopefully these interference issues can be resolved in the next five years.

From a technical perspective, we have planned the following short-term projects (in the next 12 months) to improve the usability of the beamline and endstations as well as increase productivity.

1. Load-lock upgrade of the APPES endstation, which will reduce sample change time from more than 1 hour (one sample at a time) to less than 10 minutes (at least 3 samples in the new load-lock)
2. Upgrade controls of APPES endstation components such as manipulator motors, sputtering, and gas dosing to enable automation and improve user friendliness
3. Monochromator cooling water temperature control to stabilize photon energy
4. Cleaning C contamination from the beamline optics to improve the quality of C K-edge spectra
5. Inclusion of two photodiodes within APPES chamber: One facing the sample, to measure total fluorescence yield (TFY) spectra, and one in the path of the beam at the back of the chamber, to measure asynchronous I_0 signals or XAS spectra of gases in transmission

In addition, a new IO-XAS chamber will be installed to replace the current one. The new chamber, which is expected to arrive by December 2018, will allow us to install the *in situ* cells and improve the versatility of the endstation through future additions, e.g. an electron analyzer for XPS and PEY-XAS measurements. The liquid flow cell has arrived from the ALS and it will be installed in the new IO-XAS chamber in early 2019. Technical commissioning is expected to commence in spring 2019 and it will be available for science commissioning in summer/fall 2019. The gas reactor cell is in the final development stages at the ALS.

Other future projects that require more time, cost, and resources include:

1. Upgrade sample heating in the APPES endstation to a quartz-guided IR-based heating. This heating system is more superior than the current in-vacuum ceramic button heater or pyrolytic boron nitride heater since it is completely separated from the gas environment in the chamber, so it prevents undesirable effects such background catalytic reaction and degradation of the heater due to oxidation.
2. Upgrade the sample transfer system in the APPES endstation to the more user-friendly and automatable system implemented at other soft X-ray beamlines (ESM and SIX).

Multi-modality has become increasingly important in modern scientific research. Complementary information from multiple experimental techniques under *in situ* and *operando* conditions is necessary to gain a cohesive understanding of the structure-function relationship of the material under real working conditions. It is crucial that these multiple techniques be employed to study the same system under the same experimental conditions. In addition, high-throughput experiments performed on a faster time scale are critical for monitoring the evolution of the chemical, physical, and electronic states of the system in real time. To meet these needs, a longer-term plan for the beamline involves constructing a new endstation that combine AP-XPS, XAS, IR, and XES/RIXS. IR spectroscopy is highly sensitive to chemical bonds and can provide much more detailed information about surface species that cannot be obtained with XPS or XAS. XES/RIXS provides information such as the nature of adsorbate-substrate bonding, charge transfer, oxidation state of metals, and when combined with XAS, band gap of the material.

The new endstation, called INSPIRE, evolved from the original proposal for QIX (Quick Inelastic X-ray Scattering) submitted during the beamline development proposal process in 2016, which was then approved although not yet funded. During the conceptual design meetings for QIX, we realized the advantages of combining QIX with AP-XPS and IR, not only for the scientific reasons described previously, but also because the tightly focused and high flux beam required for QIX will also be important for increasing the operating pressure and time resolution of AP-XPS experiments. In addition, by placing INSPIRE at IOS, we will benefit from proximity to the future neighboring INF IR beamline to enable the use of synchrotron IR in simultaneous AP-XPS/IR and RIXS/IR experiments. This is important for exploiting the higher brightness and broader spectral range of synchrotron IR source, which would not be possible with any conventional IR source. Finally, the design of INSPIRE with modularity and automation in mind will provide us with a modern, user friendly endstation that is urgently needed to replace the rapidly aging CFN-provided APPES endstation. Depending on the level of funding, INSPIRE can be designed and constructed in phases, starting with the AP-XPS and IR capabilities, followed by upgrades to the beamline optics and the development of the RIXS spectrometer.

Beamline Self-Assessment

So far, IOS as a beamline has been productive in terms of growth of user community and publications output. At the writing of this report, the beamline has produced 17 publications in 2018, three of which are in high impact journals (impact factor >6). The continuously increasing number of submitted proposals shown in Fig. 2 reflects the growing potential user community. Despite the productivity, there is still a lot of unfulfilled potential. First, it is difficult to meet the increasing demand for beam time due to the reduced available user time. Second, the lack of upgrades to the APPES endstation puts the beamline at a disadvantage in this constantly evolving technique compared to other beamlines running AP-XPS in other synchrotrons in the US and internationally. The age of the endstation has also made for a series of catastrophic equipment failures of late, most notably the breakdown of the electron analyzer noted earlier. However, the beamline staff have been able to offer other capabilities to affected users, thus keeping the beamline operating. As described above, we have stretched the beamline operating budget as far as possible in order to plan minor upgrades to the endstation, which improve usability and productivity. However, a long-term, more sustainable plan to make the beamline more technically and scientifically competitive in the national and global stage would be to develop the INSPIRE endstation described above as the main endstation at IOS.

Appendix A

Interference Issues at 23-ID Beamlines

The 23-ID-2 beamline has undergone a change in scientific and technical scope since its initial construction. Initially intended for fast polarization switching in XMCD experiments for condensed matter physics, the focus of the beamline has shifted to soft X-ray spectroscopy for in situ and operando chemistry using ambient pressure XPS and XAS. The SAC approved this change in 2016.

As mentioned in the Beamline Overview section, the two EPU's can be operated in the canted configuration to produce two beams, one to each of the 23-ID beamline, CSX and IOS. In theory, both beamlines can be operated simultaneously in this mode. However, after an extensive joint-commissioning, it was discovered that the small canting angle (0.16 mrad) introduces interferences in terms of photon contamination (i.e. some of CSX photons make their way to IOS, and vice versa) as well as heat load on the optics (i.e. CSX first mirror receives heat load from IOS photons). Experiments at CSX that require beam stability and coherence, in particular, suffer from interferences produced by changes in the undulator gap at IOS, which are necessary for photon energy changes on a spectroscopy beamline.

Different modes of operation were tested to minimize the effect from interferences. First, we split the operating schedule on a 12-hour basis per day, with one beamline as the controlling/driving beamline for 12 hours while the other operates in a parasitic mode, with restrictions (e.g. no changes to the undulator gap, and therefore photon energy) determined by the controlling beamline. However, this mode was found to be insufficient in relieving the effect of heat load in the optics since it can take hours for the optics to stabilize. Currently, CSX and IOS split the operating schedule 50-50 on a per user group basis, i.e. when one beamline runs a GU experiment, the other does not. In the canted mode, the beamline running a GU experiment has control of both EPU's and the other beamline can be operated parasitically for commissioning or testing purposes. Therefore, each beamline effectively operates 50% of the time. In addition, due to an incomplete electron beam position monitor (eBPM) setup, which further contributes to the overall beam instability issues, experiments at CSX that require absolute stability are performed with the EPU's in the straight mode, with no beam provided to IOS.

A working group was formed consisting of Claudio Mazzoli (CSX Lead Scientist), Ira Waluyo (IOS Lead Scientist), Joe Dvorak (soft X-ray group optics scientist), Daniel Bacescu (beamline engineer), and Julian Adams (project manager) to analyze the situation and suggest a possible solution to these interference issues. The group came to the conclusion that, short of moving one beamline to a different straight section, the best solution is to increase the canting angle from 0.16 to 2 mrad, which will eliminate the interferences. Naturally, this proposed solution comes with cost and down time for both beamlines, but in the long term it will maximize the performance of and provide 100% user operation to both CSX and IOS.

Appendix B

Complete list of users

Cycle	Last Name	First Name	Email	Affiliation
2015-3	Barbour	Andi	abarbour@bnl.gov	Brookhaven National Laboratory
	Boscoboinik	Jorge	jboscoboinik@bnl.gov	Brookhaven National Laboratory
	Kaznatcheev	Konstantine	kaznatch@bnl.gov	Brookhaven National Laboratory
	Mazzoli	Claudio	cmazzoli@bnl.gov	Brookhaven National Laboratory
	Palomino	Robert	rpalomino@bnl.gov	Brookhaven National Laboratory
	Waluyo	Iradowikanari	iwaluyo@bnl.gov	Brookhaven National Laboratory
	Wilkins	Stuart	swilkins@bnl.gov	Brookhaven National Laboratory
	Zhong	Jianqiang	jzhong@bnl.gov	Brookhaven National Laboratory
2016-1	Akter	Nusnin	nusnin.akter@stonybrook.edu	SUNY @ Stony Brook
	Barbour	Andi	abarbour@bnl.gov	Brookhaven National Laboratory
	Boscoboinik	Jorge	jboscoboinik@bnl.gov	Brookhaven National Laboratory
	Broderick	Alicia	Johnstoa@udel.edu	University of Delaware
	Carpena-Nunez	Jennifer	jennifercarpena@gmail.com	Brookhaven National Laboratory
	Chen	Zhu	zc@princeton.edu	Princeton University
	Grinter	David	dgrinter@bnl.gov	Brookhaven National Laboratory
	Kaznatcheev	Konstantine	kaznatch@bnl.gov	Brookhaven National Laboratory
	Kestell	John	jkestell@bnl.gov	Brookhaven National Laboratory
	Kronawitter	Coleman	colemank@princeton.edu	Princeton University
	Li	Chaoran	chaoran.li.89@gmail.com	Binghamton University, SUNY
	Liu	Qianqian	qliu16@binghamton.edu	Binghamton University, SUNY
	Luo	Si	nju07luosi@gmail.com	SUNY @ Stony Brook
	Mazzoli	Claudio	cmazzoli@bnl.gov	Brookhaven National Laboratory
	Mullins	David	mullinsdr@ornl.gov	Oak Ridge National Laboratory
	Nguyen	Luan	lnguyen7@nd.edu	University of Kansas
	Overbury	Steven	overburysh@ornl.gov	Oak Ridge National Laboratory
	Palomino	Robert	rpalomino@bnl.gov	Brookhaven National Laboratory
	Rani	Sana	srani@udel.edu	University of Delaware
	Saber	Sammy	sammy.saber.ctr@us.af.mil	UES, Inc.
	Stacchiola	Dario	djs@bnl.gov	Brookhaven National Laboratory
	Stach	Eric	estach@bnl.gov	Brookhaven National Laboratory
	Waluyo	Iradowikanari	iwaluyo@bnl.gov	Brookhaven National Laboratory
	Wilkins	Stuart	swilkins@bnl.gov	Brookhaven National Laboratory
	Xu	Fang	fangxu@bnl.gov	Harvard University
	Yao	Siyu	siyuyao@bnl.gov	Brookhaven National Laboratory
	Zakharov	Dmitri	dzakharov@bnl.gov	Brookhaven National Laboratory
	Zhang	Shiran	szhang5@nd.edu	Massachusetts Institute of Technology (MIT)
	Zhao	Peng	pztwo@princeton.edu	Princeton University
	Zhong	Jianqiang	jzhong@bnl.gov	Brookhaven National Laboratory
	Zhou	Guangwen	gzhou@binghamton.edu	Binghamton University, SUNY
	2016-2	Akter	Nusnin	nusnin.akter@stonybrook.edu

Avincola	Valentina	valentina.avincola@kit.edu	University of Virginia
Barbour	Andi	abarbour@bnl.gov	Brookhaven National Laboratory
Boscoboinik	Jorge	jboscoboinik@bnl.gov	Brookhaven National Laboratory
Bruce	Jared	jpbruce@uci.edu	University of California @ Irvine
Chen	Zhu	zc@princeton.edu	Princeton University
Galhenage	Randima	rgalhen@uci.edu	University of California @ Irvine
Garrido Rodriguez	Isamar	isamargarrido1@gmail.com	Hostos Community College
Goldsbrough	Roger	roger@quantumdetectors.com	Quantum Detectors
Grinter	David	dgrinter@bnl.gov	Brookhaven National Laboratory
Hamlyn	Rebecca	rebecca.hamlyn@stonybrook.edu	SUNY @ Stony Brook
Hunt	Adrian	adhunt@bnl.gov	Brookhaven National Laboratory
Jimenez Divins	Nuria	nuria.divins@gmail.com	Ruhr-Universitat Bochum
Kestell	John	jkestell@bnl.gov	Brookhaven National Laboratory
Li	Chaoran	mithrilf91@gmail.com	Binghamton University, SUNY
Lin	Zhexi	zl2453@columbia.edu	Columbia University
Liu	Qianqian	qliu16@binghamton.edu	Binghamton University, SUNY
Liu	Zongyuan	liuzongyuan1988@gmail.com	Brookhaven National Laboratory
Lu	Qiyang	qiyanglu@mit.edu	Oak Ridge National Laboratory
Luo	Si	nju07luosi@gmail.com	SUNY @ Stony Brook
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Appendix C

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1. J. P. Simonovis, A. Hunt, S. D. Senanayake, I. Waluyo, Subtle and Reversible Interactions of Ambient Pressure H₂ with Pt/Cu(111) Single Atom Alloy Surfaces, *Surf. Sci.* (2018). DOI: 10.1016/j.susc.2018.09.003
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