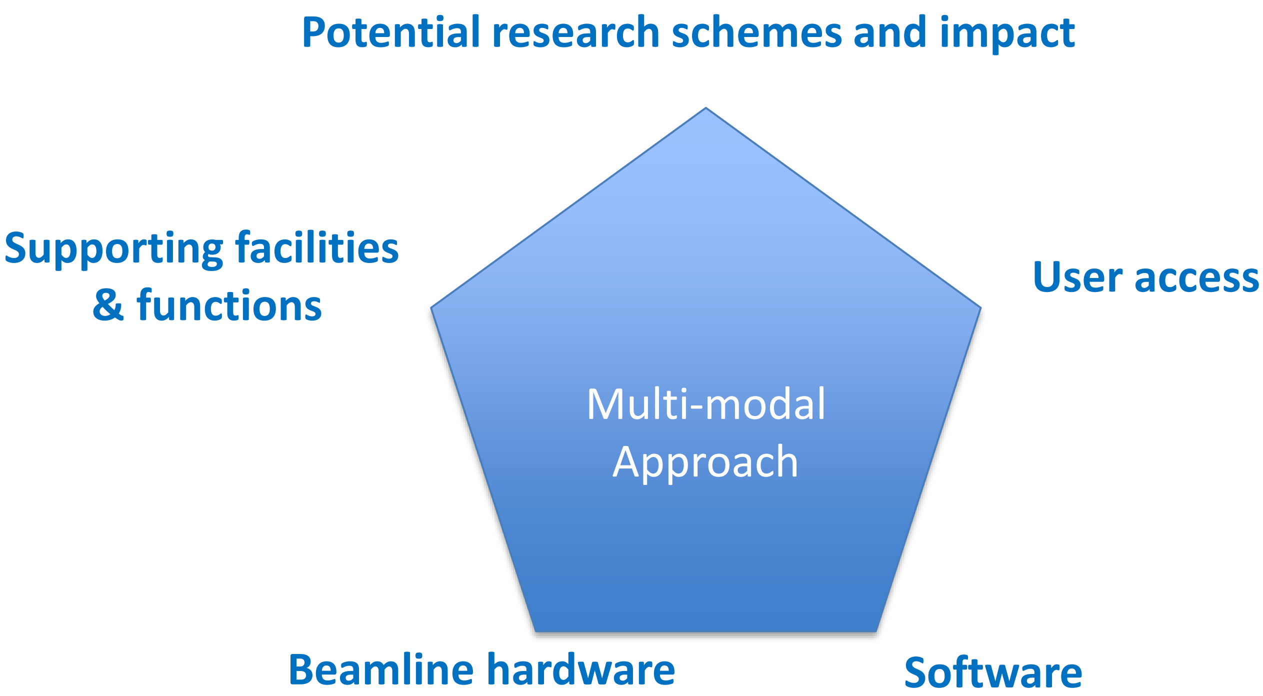
# Multi-modal Issue Task Force
## March 1, 2017
## UEC Town Hall Meeting

Yu-chen Karen Chen-Wiegart, Yong Chu, Eric Dooryhee, Klaus Attenkofer, Lisa Miller, Iradwikanari Waluyo, Daniel Allan, Lin Yang, Wah-Keat Lee, Randy Smith, Stuart Campbell

# Charter & Role

The Multi-Modal Issues Task Force (MMITF) is established to identify the issues involved in **utilizing techniques across multiple beamlines** at NSLS-II, and in combining synchrotron techniques with **other techniques, such as the electron-based imaging methods at CFN**. The task force shall not aim to fully resolve the issues, but rather to **clearly identify them, assign priorities to addressing them and provide suggested paths forward** in each case.




Goal

Logistics

Techniques

# Task force members

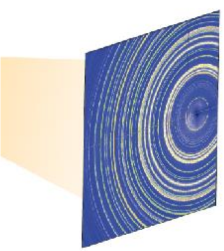
| Member | |
|---|---|
| **Karen Chen-Wiegart** | Chair - under joint appointment, with Mat Sci & Chem. Eng, SBU |
| **Yong Chu** | Lead Scientist, Hard X-ray Nanoprobe beamline |
| **Eric Dooryhee** | Program Manager, Diffraction & In Situ Scattering<br>Lead Scientist, X-Ray Atomic Pair Distribution Function & X-Ray Powder Diffraction |
| **Klaus Attenkofer** | Program Manager, Hard X-Ray Spectroscopy 8-ID<br>Lead Scientist, Inner Shell Spectroscopy |
| **Lisa Miller** | Program Manager, Imaging & Microscopy<br>Users program; Users Issues Task Force Chair |
| **Iradwikanari Waluyo** | Lead Scientist, Soft X-ray Spectroscopy & Polarization |
| **Daniel Allan** | Assistant Computational Scientist, Data Acquisition, Management and Analysis |
| **Lin Yang** | Lead Scientist, Life Science X-ray Scattering |
| **Wah-Keat Lee** | Lead Scientist, Full-Field X-ray Imaging |
| **Randy Smith** | Laboratory Space Manager; Science Associate |
| **Stuart Campbell** | Group Leader, Data Acquisition, Management and Analysis |

# Responsibilities

**1. Potential research schemes and impact:** to identify scientific cases and communities in which techniques and beamlines may be usefully combined and the impact of doing so.

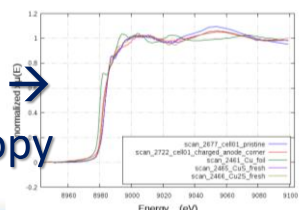
**1) Complex systems:** science cases require combining different interaction mechanisms to fully understand the systems.
**2) Hierarchical, heterogeneous structure:** science cases require a particular interaction mechanism but at different length scales.

Morphology
→ imaging



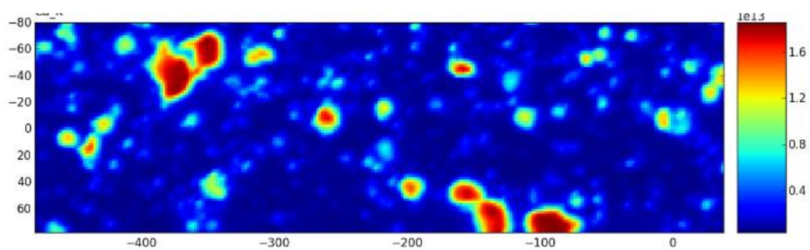
Structure
→ diffraction
& scattering

Chemistry →
spectroscopy

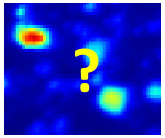



**Complex**

**Heterogeneous**

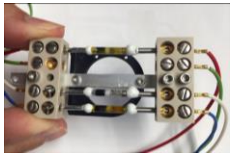



*Li-S battery with CuS addtives*




Particles
(material)

Clusters
(Electrodes)

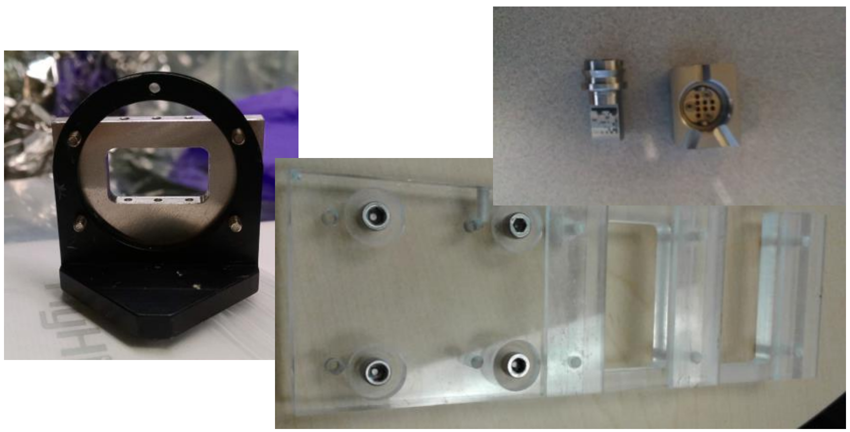


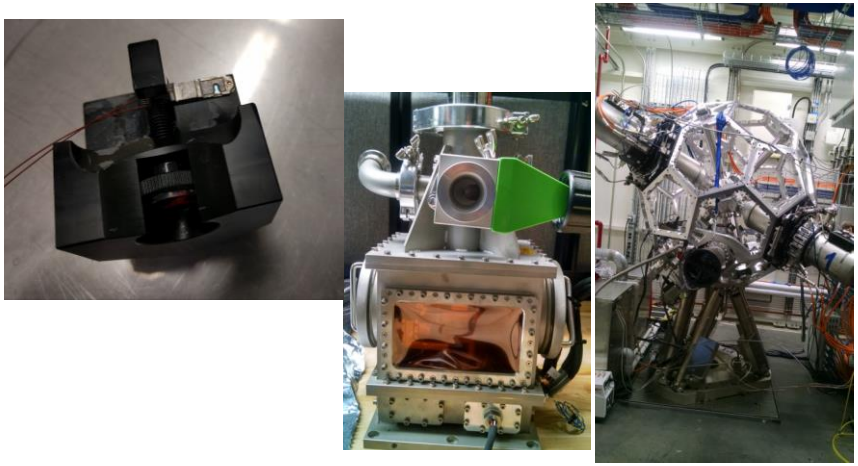
Interfaces & Devices
(System)

# Responsibilities (con't)

**Type of multi-modal measurements**

1) **Static samples:** the exact same samples need to be measured across different beamlines without physical changes: simple and fast sample registration between beamlines and laboratory techniques is critical.





***2) In operando/In situ* experiments:** *in situ* cells need to be compatible across different beamlines in order to create the same *operando* conditions. The development of software that provides the ability to align and analyze *operando* data measured from different beamlines and techniques is required.

# Responsibilities (con't)

**Identify the issues required for an effective multimodal program in:**

**Beamline hardware:**
- Identify sample mounting/geometry requirements
- standard form factor sample cells
- sample environment control
- common equipment and stages

**Software:**
- Data acquisition
- Data Registration
- Data Analysis
- Data Visualization
- Data Access
- Data Modeling

**User access**
- Proposal submission and review
- Beamtime allocation
- Cross-facility proposal system & time allocation

**Supporting facilities and functions:**
- Support lab access
- User training/education/out-reach

# Resources & Reporting

- The MMITF is assigned no special resources, but has the authority to provide recommendations to the NSLS-II Division Directors and NSLS-II Director on funding projects and requests, as needed. The NSLS-II Facility Director has final decision and approval authority on resource allocations.

- A written report is due every half a year (Jan and June)

# Conduct of the task force: Launched October 26, 2016

| Date | Topic | Action Items |
|---|---|---|
| 01 – 10/28/2016 | Strategic Report Write-up Kick-off | Individuals assigned sections |
| 02 – 11/04/2016 | Strategic Report 2nd Iteration | Individuals will review draft<br>Hardware survey: Randy Smith<br>Software survey: Dan Allan |
| 03 – 12/05/2016 | Hardware Needs – I<br>User Access - I | Continue Hardware survey<br>(8 out of 18 operational BLs done) |
| 04 – 12/12/2016 | Software Needs - I<br>User Access – II | Continue Software survey<br>(12 out of 18 operational BLs done) |
| 05 – 01/25/2017 | SPMC* presentation draft | → Update by April |
| 06 – 02/15/2017 | SPMC presentation feedback | Address SPMC discussions |

**Science Programs Management Committee*

**Mechanisms of documentations:**

- **Strategic Plan:** all contributed to the write-up
- **All meetings are documented on SharePoint:**
  Attendees, Agenda, Presentation Slides (including discussion notes)

# Beamline Survey Status – Hardware & Software

| Beamline | Hardware | Software |
|---|---|---|
| | | |
| **Operational/Comissioning Beamlines (18)** | (8) | (12) |
| 3-IDHard X-ray Nanoprobe(HXN) | v | v |
| 4-IDIntegrated In-situ and Resonant Hard X-ray Studies(ISR) | | |
| 5-IDSubmicron Resolution X-ray Spectroscopy(SRX) | v | v |
| 8-BMTender Energy X-ray Absorption Spectroscopy(TES) | v | v |
| 8-IDInner-Shell Spectroscopy(ISS) | v | v |
| 10-IDInelastic X-ray Scattering(IXS) | | |
| 11-BMComplex Materials Scattering(CMS) | v | v |
| 11-IDCoherent Hard X-ray Scattering(CHX) | v | v |
| 12-IDSoft Matter Interfaces(SMI) | | v |
| 16-IDLife Science X-ray Scattering(LIX) | v | v |
| 17-BMX-ray Footprinting for In Vitro and In Vivo Structural Studies of Biological Macromolecules(XFP) | | |
| 17-ID-1Highly Automated Macromolecular Crystallography Beamline(AMX) | | |
| 17-ID-2Frontier Microfocusing Macromolecular Crystallography(FMX) | | |
| 19-IDBiological Microdiffraction Facility(NYX) | | |
| 21-IDElectron Spectro-Microscopy(ESM) | | v |
| 23-ID-1Coherent Soft X-ray Scattering(CSX-1) | | v |
| 23-ID-2Soft X-ray Spectroscopy and Polarization(CSX-2) | | v |
| 28-ID-2 X-ray Powder Diffraction(XPD) | v | v |
| | | |
| **Beamlines Under Development (10)** | (2) | (2) |
| 2-IDSoft Inelastic X-ray Scattering(SIX) | | |
| 4-BMX-ray Fluorescence Microprobe(XFM) | v | V |
| 6-BMMaterials Measurement(BMM) | | |
| 7-BMQuick x-ray Absorption and Scattering(QAS) | | |
| 7-ID-1Spectroscopy Soft and Tender(SST-1) | | |
| 7-ID-2Spectroscopy Soft and Tender(SST-2) | | |
| 18-IDFull Field X-ray Imaging(FXI) | v | V |
| 22-BM-1Frontier Synchrotron Infrared Spectroscopy(FIS) | | |
| 22-BM-2Magnetospectroscopy, Ellipsometry and Time-Resolved Optical Spectroscopies(MET) | | |
| 28-ID-1Total Scattering Beamline(PDF) | | |
| 27-ID (HEX): High Energy X-ray Diffraction | | |

| Program | Hardware | Software |
|---|---|---|
| Hard X-Ray Spectroscopy (6) – Eric | (3) | (3) |
| Soft X-Ray Scattering & Spectroscopy (5) – Karen – 2, 21-23; Eric – 2*2 | (0) | (3) |
| Imaging & Microscopy (4) – Karen | (4) | (4) |
| Complex Scattering (4) – Jianming | (2) | (3) |
| Structural Biology (5) – LiX only - Karen | (1) | (1) |
| Diffraction & In Situ Scattering (4) – Jianming | (1) | (1) |

- **Lead on survey/discussions**

**Hardware:** Randy Smith

**Software:** Dan Allan

| Beamline | Hardware | Software |
|---|---|---|
| Operational/ Commissioning Beamlines (18) | 8 | 12 |
| Beamlines Under Development (10) | 2 | 2 |

# Hardware: focusing on sample mounting constraints & compatibility

Summarizing information in spreadsheet

| be | beamline | station/mode | beam size/res | techniques | typical sample mounting | limitations | working distance from beam focus | compatable substrates/ windows | energy range | likely multimodal partner | mapping stage? Mapping sofware |
|---|---|---|---|---|---|---|---|---|---|---|---|
| B | 02-ID SIX | | 6x0.6 microns | soft inelastic x-ray scattering | | | | | | | |
| B | 03-ID HXN | MLL | 20nm | hard X-ray Flourescence, diffraction | 2D:custom mount only ("diving board"), 3D: custom tomo mount | in-vacuum, no working distance | mm | | 6-25KeV | | yes, yes |
| B | 04-BM XFM | main | 1-2 micron | hard X-ray Flourescence, XANES | 2D: 2"x2" flat mount 45 deg tilt, tomo: Huber goniometer (2" tall + pin) | small working distance- 60mm upstream | upstream: 60mm | ultralene, kapton, | 2-23KeV | TES, SRX, HXN (BMM, QAS, & ISS for bulk) | yes, yes |
| B | 04-ID ISR | | 2x20 microns | scattering and diffraction | | | | | | | |
| B | 05-ID SRX | high flux | < micron | hard X-ray Flourescence, point XANES | 1" diameter magnetic mount typicall 15 deg(?) tilt, w/ different attaching plates | ~ 5 - 10 mm working distance to in-line optical microscope | upstream, 5-10 mm w/ in-line microscope | | 4.7-25KeV | | |
| B | 08-BM TES | main | 10 micron to 1mm | tender X-ray Flourescence | 2"x2" flat mount, 45 deg tilt | He atmosphere, ultralene substrate | | | 1-8KeV | XFM, SRX, HXN (BMM, QAS, & ISS for bulk) | yes, yes |
| B | 08-ID ISS | soccerball station | 1mm^2 or 20-25um | XAFS, XANES, X-ray Flourescence | 10 sample chages w/ electrical and gas feed through | must be mounted on stanard mount | | Kapton, other polymers | 2.5-36KeV | | |
| B | 08-ID ISS | standard XAFS | 1mm^2 up to 3x60mm | XAFS, XANES, X-ray Flourescence | translation stage w/ lots of flexibility. Typical 13mm pressed pellets | | ISS | Kapton, other polymers | 2.5-36KeV | | |
| B | 10-ID IXS | | 5x7 microns | Inelastic Scattering | | | | | | | |
| B | 11-BM CMS | main | 200x200 microns typical (min 20x20 um) | SAXS/WAXS | 1. cabilary 1mm glass or quartz 2. G.I- thin film 1x1cm x10 samples (1" thorlabs mount, vacuum compatable) | | centimeters (upstream and downstream) | Kapton (8 or 25 microns) | 10-17KeV | 1. CHX, LIX, SMI 2. Spectroscopy & imaging beamlines | yes, ? |
| B | 11-ID CHX | | 3 & 10 microns | SAXS/WAXS, Correlated Spectroscopy | 1. capilaries (10 um wall) & flow cells 2.custom for wafers, gels, (transmission & reflection geomatery) | | | | 6-16KeV | 1. CMS, 2. SMI | yes, ? |
| B | 12-ID SMI | | 2.5x25micron | GI SAXS/WAXS | | | | | | | |
| B | 16-ID LiX | main | 1 to 500 microns | SAXS/WAXS (solution and microprobe) | 1. solutions (200-30uL in 200uL PCR tube) flow cell and non-flow cell 2. thin sample 3D mapping | microprobe: ~5mm tall, 10-100 microns thick. Solution:30-200uL | upstream ~30mm downstream ~ 3 mm | | 2-18 KeV | crystalograpny beamlines, microprobe imaging techniques, solution XAS | yes, ? |

beamline vs spot size | Sheet3

& in presentation (photos, comments)

Drawings are also collected

**On-going efforts by Randy Smith**

LiX – SAX/WAX (2-18KeV)

**Two sample types/ beamline modes:**

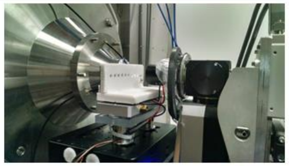
1. Solutions
   - Flow cell: 200-30uL in PCR tube
   - No-flow cell
   - HPLC effluents
2. 2D samples: microprobe setup
   - 1um beam
   - Mapping stage, ~5mm flat samples
   - Visible light microscope (10x)

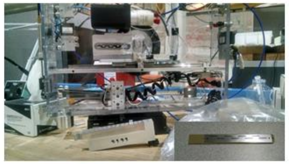
**Constraints (microprobe):**

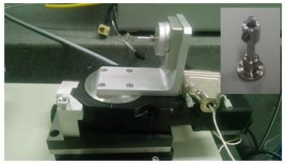
- ~5mm sample or smaller
- upstream working distance 33mm (lens)
- downstream working distance 3mm (scatter cone)

**Likely multimodal partners:**

- Crystallography beamline (AMX,FMX, NYX)- studying particular protein or molecule
- All modes of imaging/microprobes (SRX, TES, XFM, IR microscopy, lab-based microscope)



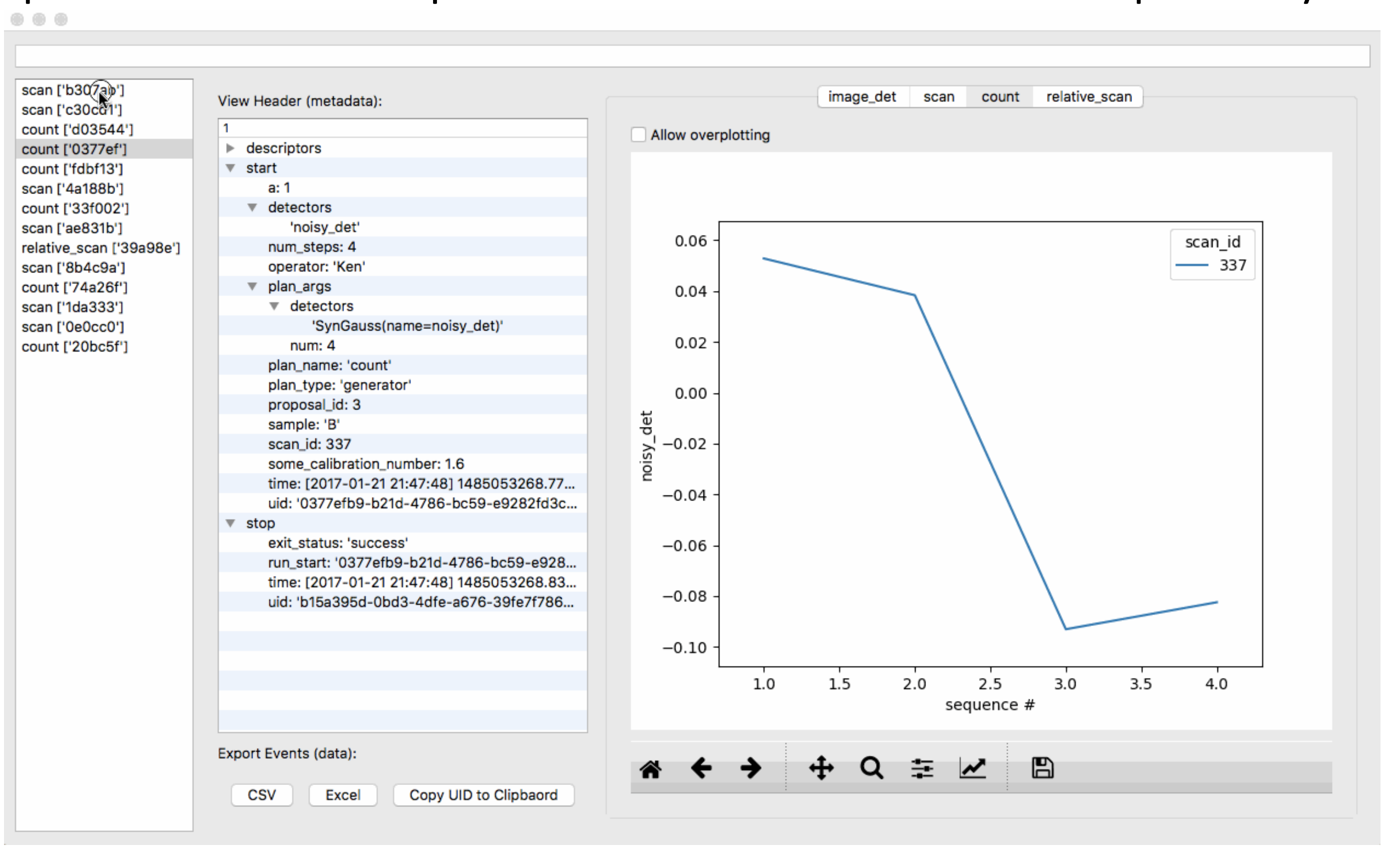




# Software: synergy with other beamlines - Two Modes of Sharing

1. Sharing actual samples and data
2. Sharing some common data acquisition and analysis code

Example: data viewer compatible across beamlines – in development by Dan Allan




**On-going efforts by Dan Allan**

# Recommendations

## 1. Proposed pilot programs directions

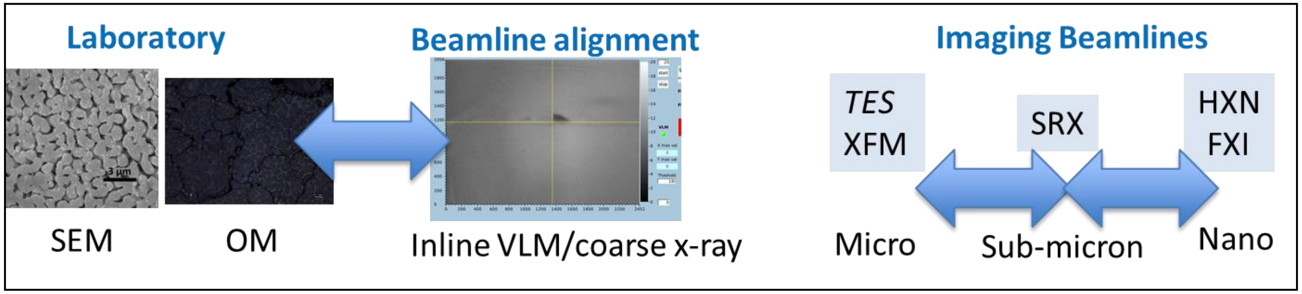
### A. Establishing end-to-end beamline hardware & software in multi-modal mode

I. Registration across beamlines: imaging beamlines

II. Sample mounting & data sharing between high throughput to specialized beamlines

### B. Science driven complex multi-modal characterization and analysis

- batteries: Li-S battery, with SRX, ISS, XPD → TES, HXN → TEM (CFN)
- catalysis, corrosion, bio-fuels, others



# Recommendation (con't)

## 2. Multi-beamline proposal (still in discussions)

- Proposal submission, review and allocation mechanism are in discussions
- Guidelines for PASS developer
- Identifying scientific opportunities  from users community

| | |
|---|---|
| **Goals** | 1. Streamline the process better to encourage/facilitate experiments take advantage of multi-modal approach to enhance the research<br>2. It has to be EASIER for the USERS |

Multi-modal proposal

↓

Multi-modal panel
(members/chairs from panel A, B, C)

↓

Allocations

*Common scientific section (project)
individual sections for each beamline request

*proposal needs to specify → allocation
1. Dependency between techniques A, B & C
2. Required order (if any) for techniques A, B & C

# Task force looking forward

- Continue to address:

1. Establishing end-to-end beamline hardware & software in multi-modal mode → start planning & aim to conducting pilot experiment(s) in 2nd & 3rd cycle of 2017
2. Exploring science driven complex multi-modal characterization and analysis, starting to engage partners/collaborators → started on Li-S battery, seeking partnership for other areas
3. Continuing discussions on multi-modal proposal mode → aim to have trial proposal for the fall cycle with details currently in discussions

- Look for feedbacks & engagement from beamline staff, groups - mechanical engineering, control engineering, DAMA, and potential partners/collaborators/users

# Looking for feedbacks from UEC

- Scientific ideas/opportunities that would benefit from a multi-modal approach?
- What beamline hardware, software & supporting functions are essential to optimize the outcome when doing multi-modal experiments?
- How do you envision planning a multi-modal experiment? (Having multiple techniques sequentially or in parallel? Having one main technique with other short/supportive beamtime or multiple beamtime with similar importance?)
- Specifically in the contents of pilot programs – looking for suggestions on samples ideal for multi-modal imaging

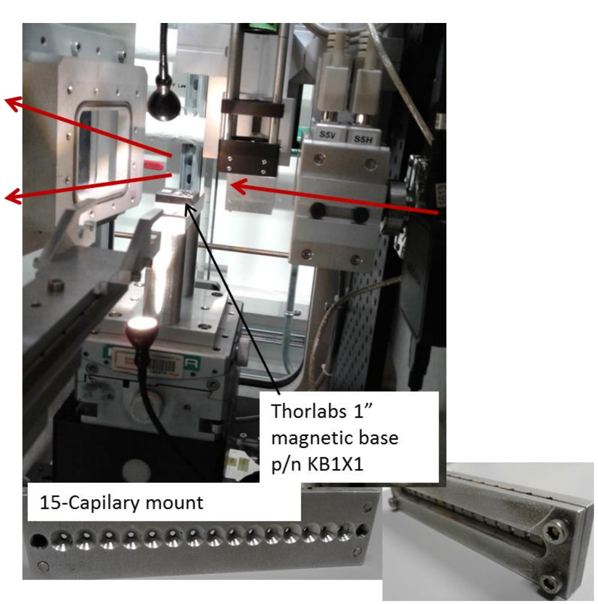
**ycchen@bnl.gov → also feel free to contact any of us:**

Yu-chen Karen Chen-Wiegart, Yong Chu, Eric Dooryhee, Klaus Attenkofer, Lisa Miller, Iradwikanari Waluyo, Daniel Allan, Lin Yang, Wah-Keat Lee, Randy Smith, Stuart Campbell

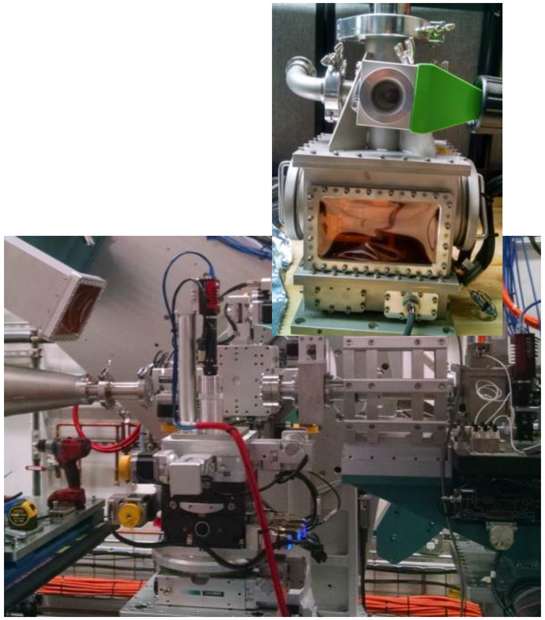
# Additional Information

# Pilot programs: A Establishing end-to-end beamline hardware & software in multi-modal mode

## 2. Sample mounting & data sharing between high throughput to specialized beamlines: scattering beamlines (start from CMS → CHX)



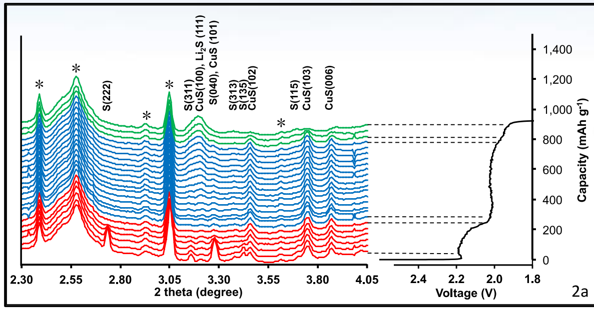

**CMS**
High throughput



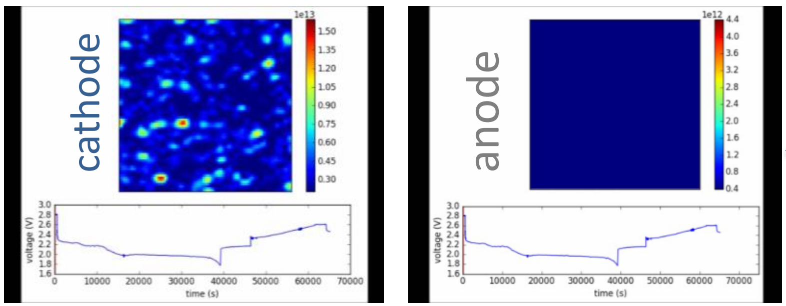
**CHX**
Specialized (dynamic)

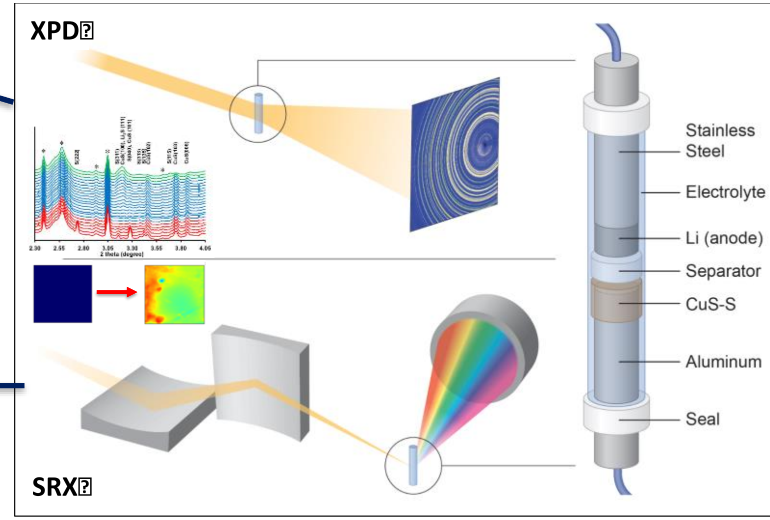
1. Hardware: compatible sample mount from CMS to CHX
2. Software: being able access *processed data* of CMS at CHX
   (check consistency between CMS and static data collected at CHX),
consistent SAXS data analysis package, sample tracking/meta data policy

# Pilot programs: B. Science driven complex multi-modal characterization and analysis - 1. batteries: Li-S battery




Open questions on data merging & correlation




**Purpose of Multi-modal Synchrotron Characterizations:**

XRF mapping for **elemental distribution evolution** (SRX) – 2016-2

X-ray diffraction for **structure and phase-identification** (XPD) – 2016-3, 2017 Feb

Hard x-ray spectroscopy for **oxidation states and structures on metals** (ISS) - 2017 March

Tender x-ray spectroscopy for **sulfur species - 2017 April**

Nano-tomography and spectroscopic imaging for **morphological and chemical evolution** (HXN, FXI)

Small angle scattering for **longer range structural information** (CMS, LiX)

Local morphological and structural evolution with high resolution (CFN – in situ TEM)

# Discussions on Multi-beamline Proposal

| | |
|---|---|
| **Goal** | **1. Streamline the process better to encourage/facilitate experiments take advantage of multi-modal approach to enhance the research**<br>**2. It has to be EASIER for the USERS** |

**Idea - I** Multi-modal proposal

Panel A Panel B Panel C

Calibration run
(members/chairs from panel A, B, C)

Single score? Multiple score?

**Idea - II** Multi-modal proposal

Multi-modal panel
members/chairs from panel A, B, C

Single score? Multiple score?

*Common scientific section (project)
individual sections for each beamline request

*Reference to SSRL's model by sending out proposals for review?
* Having Science-oriented review panel?

*number of shifts depends on beamline

*proposal needs to specify → allocation

1. Dependency between techniques A, B & C
2. Required order (if any) for techniques A, B & C

# Issues to address

| Multi-modal aspect | Hardware – sample mounting | Software |
|---|---|---|
| 2D imaging /scanning registration | **Design compatible 2D sample mount/adaptors - **FXI, HXN, SRX, XFM, TES, LiX<br>**Plan and execute proof of concept experiment across imaging beamlines** | **Evaluate existing imaging registration utilities available in compatible environment, and apply them to the proof-of-concept experiment** (FXI, HXN, SRX, XFM, TES)<br><br>**Configure Databroker and File system to ensure data can be viewed across beamline** |
| Tomography | **Design compatible tomography sample mount/adaptors -** FXI, HXN, SRX, XFM | **Continue the efforts on tomography reconstruction software -TomoPy implementation** |
| Multi-dimensional data | | **Further establish a consensus across the facility on how to provide a visualization tools for multi-dimensional arrays s sustainable with the support of DAMA group & continue the efforts**<br>• At ESM, band structure cubes<br>• Scattering image time series at many beamlines<br>• XANES imaging stack and tomography series at imaging beamlines |

# Issues to address – con't

| Multi-modal aspect | Hardware – sample mounting | Software |
|---|---|---|
| Scattering | **Design compatible sample mount/adaptors -** high through-put (CMS) vs specialized (CHX, SMI) | 1. Bin statistics for Power Diffraction (XPD), SAXS, WAXS, GI-SAXS, GI-WAXS (CMS, CHX, SMI, LiX): **Consolidate the processing functions, and then develop a standalone GUI application**<br>2. XPCS (CHX, CSX-I): **Enhancements – moving from Jupyter (Python Notebook) to a GUI** |
| *In situ* sample holders | **Continue on-going compatible battery efforts:** SRX, XPD, ISS, potentially TES<br>**Continue on-going flow cell efforts:** SRX, HXN, and TEM (CFN)<br>**Catalysis –** start discussions with partners/collaborators in Chemistry department | |
| Multi-modal complex data | | Using scientific cases (battery, catalysis), **identify clear statistical analysis** – correlation analysis across techniques: synergy with CSI |
| High throughput experiments | Start discussions about high throughput across programs/mechanisms (ISS and XPD) | Sample tracking & meta data 'default'<br>Consistent bar-code systems (Reference: structural biology beamlines, other facilities) |