National Synchrotron Light Source II

New Strategic Plan 2019-2023

Qun Shen

Deputy Director for Science

NSLS-II

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U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKHAVEN NATIONAL LABORATORY

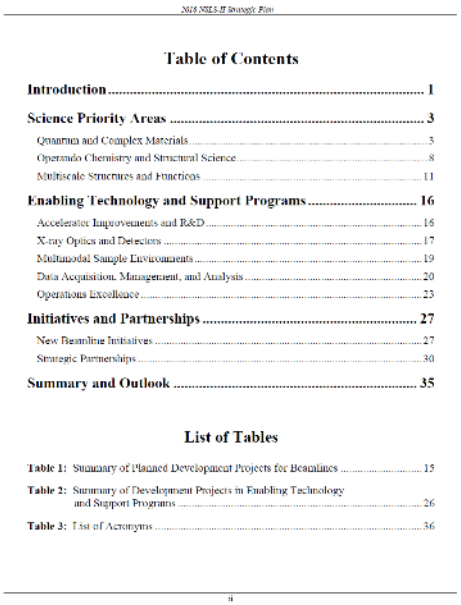
Outline

- Strategic planning process
- Accelerator plans
- Beamline programs plans
- New beamline concepts and next steps
- Summary

Continuous Strategic Planning Process

https://www.bnl.gov/ps/docs/pdf/NSLS2-Strategic-Plan.pdf

- Current NSLS-II Strategic Plan published Apr 2018, based on SAC input from previous meetings
- New guideline to publish updated facility's Strategic Plan at the beginning of new DOE fiscal year
- Thus our accelerated schedule for the new 2019-2023 Strategic Plan



2018 NSLS-II Strategic Plan

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- New five-year plan will follow similar style and contents and capture only development projects beyond normal operations, with refreshed background information and updated projected activities

Planning Process 2018

- Brainstorming sessions held for each of the technical programs, to engage more staff in the planning process
  - Development ideas and plans discussed
  - Some further discussed and feed into new Strategic Plan
- Facility improvement projects launched, with ideas solicited from staff:
  - 20 proposals received and reviewed by management; 8 approved to proceed
  - These activities also feed into new Plan

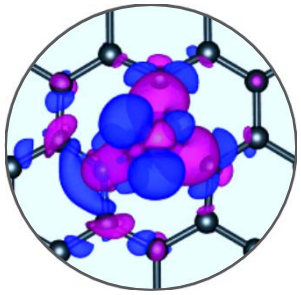
Brainstorming Sessions 2018

Controls and data	Mar 26
Experimental development	Mar 28
Diffraction & in-situ scattering	Apr 3
Soft x-ray scat & spectroscopy	May 7
Hard x-ray spectroscopy	May 9
Structural biology	May 11
Imaging & microscopy	May 18
Complex scattering	Jun 20
Accelerator – operations	Aug 15
Accelerator – development	Sep 12

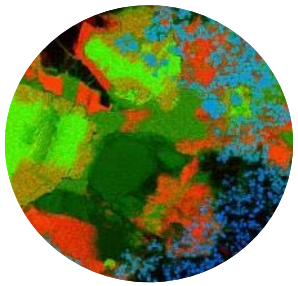
- Ideas and concepts of add'l new beamlines (*beyond the 6 approved in 2016*):
  - Solicited 2-slides for each new beamline ideas from staff
  - Beamline program managers consolidated and presented these ideas
  - Will engage SAC and user community to further discuss these in coming months

Science Focus Areas

- Quantum and Complex Materials:
  - Materials with interacting quantum states and intrinsically complex heterogeneous systems
  - NSLS-II: coherence, nano-imaging, IXS, μ-beam scattering for studies of heterogeneities & naturally-occurring dynamics and processes



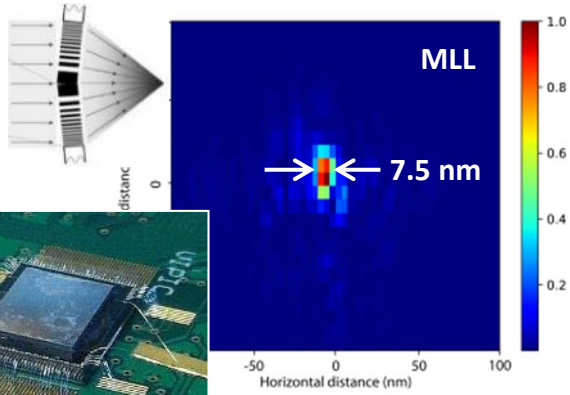
- *Operando* Structural Chemistry:
  - Understandings of how things function in real environment and under working conditions
  - NSLS-II: high intensity & hazardous gas handling for time-resolved high-throughput XAS & XRD studies in realistic operating conditions

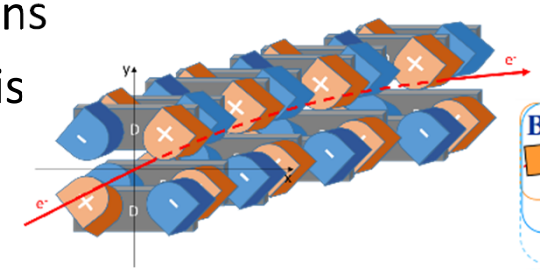


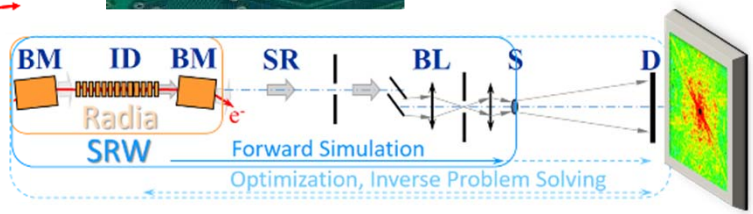
- Multiscale Structure and Function:
  - Structural, electronic, morphological, chemical, and biochemical behavior at multiple spatial and temporal scales
  - NSLS-II: cutting-edge micro-/nano-imaging and structural biology tools that span multiple length and time scales

Enabling Technologies R&D and Support

- NSLS-II R&D program:
  - Objective: to advance targeted technology areas critical to NSLS-II's mission
  - Leveraging the strengths and talents among our staff
  - Coordination with other LS facilities
- Current activities:
  - Accelerator R&D
  - X-ray optics, metrology, detectors
  - Multimodal experimental methods and simulations
  - Integrative data analysis & management, and applications of AI

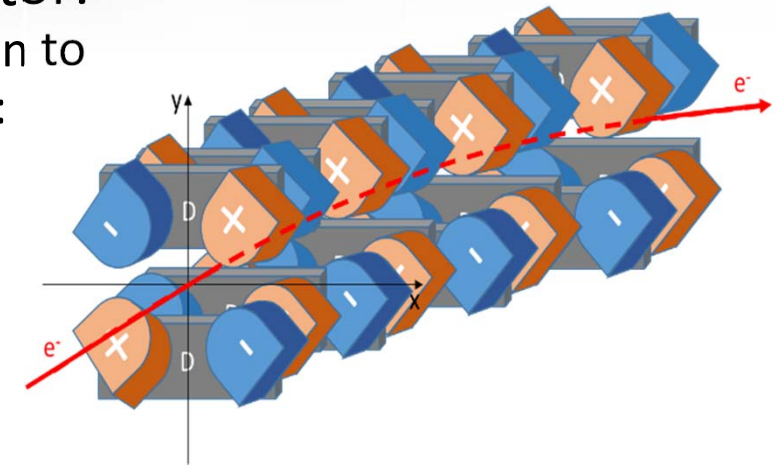




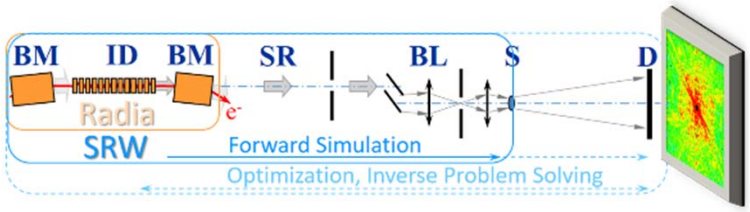


Accelerator Improvement Plan and R&D

- Continued evolution of NSLS-II accelerator:
  → essential part of the facility strategy. We plan to pursue accelerator development in three areas:
  - Developments that support reliable operations
  - Developments that are required to ramp up performance to its design specs
  - R&D that lead to enhanced or upgraded NSLS-II performance beyond design specifications

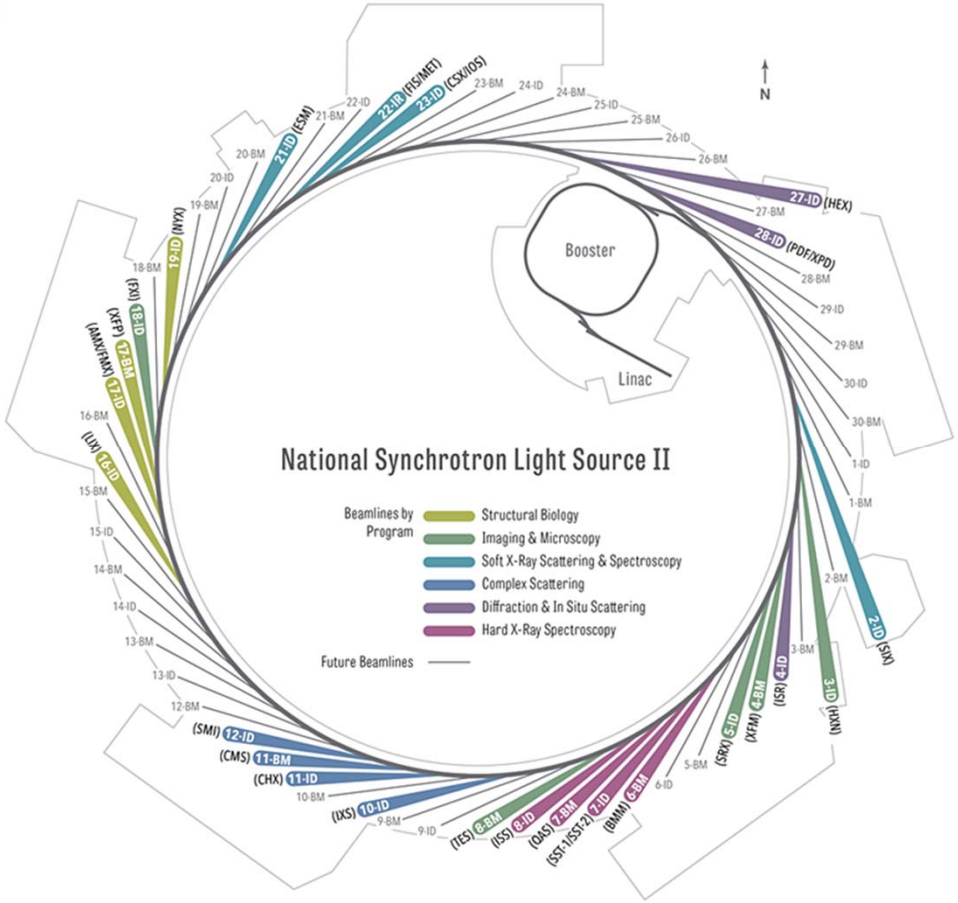


- Large scale projects in next five years:
  - 3rd and 4th RF, LINAC klystron upgrade, complete critical spares, redundant cryo-plant and other systems, harmonic cavities



  - Identify and develop high-brightness IDs best suited for NSLS-II applications
  - Simulations and modelling from source to realistic experiments
  - Develop plans for performance-effective and cost-efficient high-brightness upgrade to NSLS-II

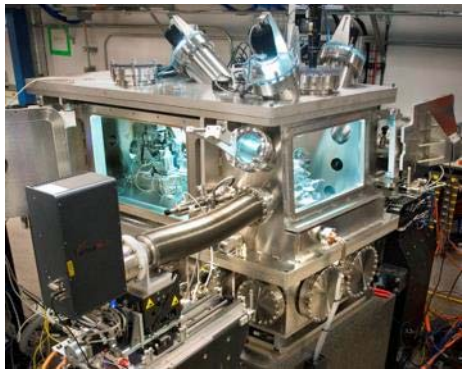
Beamline Programs



- Continue to ramp-up as-designed capabilities and mature user programs
- Increase productivity and impact by engaging in in-depth data analysis and theoretic modelling
- Mature data acquisition and data management/storage systems
- Develop and start implement improvement and upgrade plans to keep systems and capabilities at the state-of-the-art

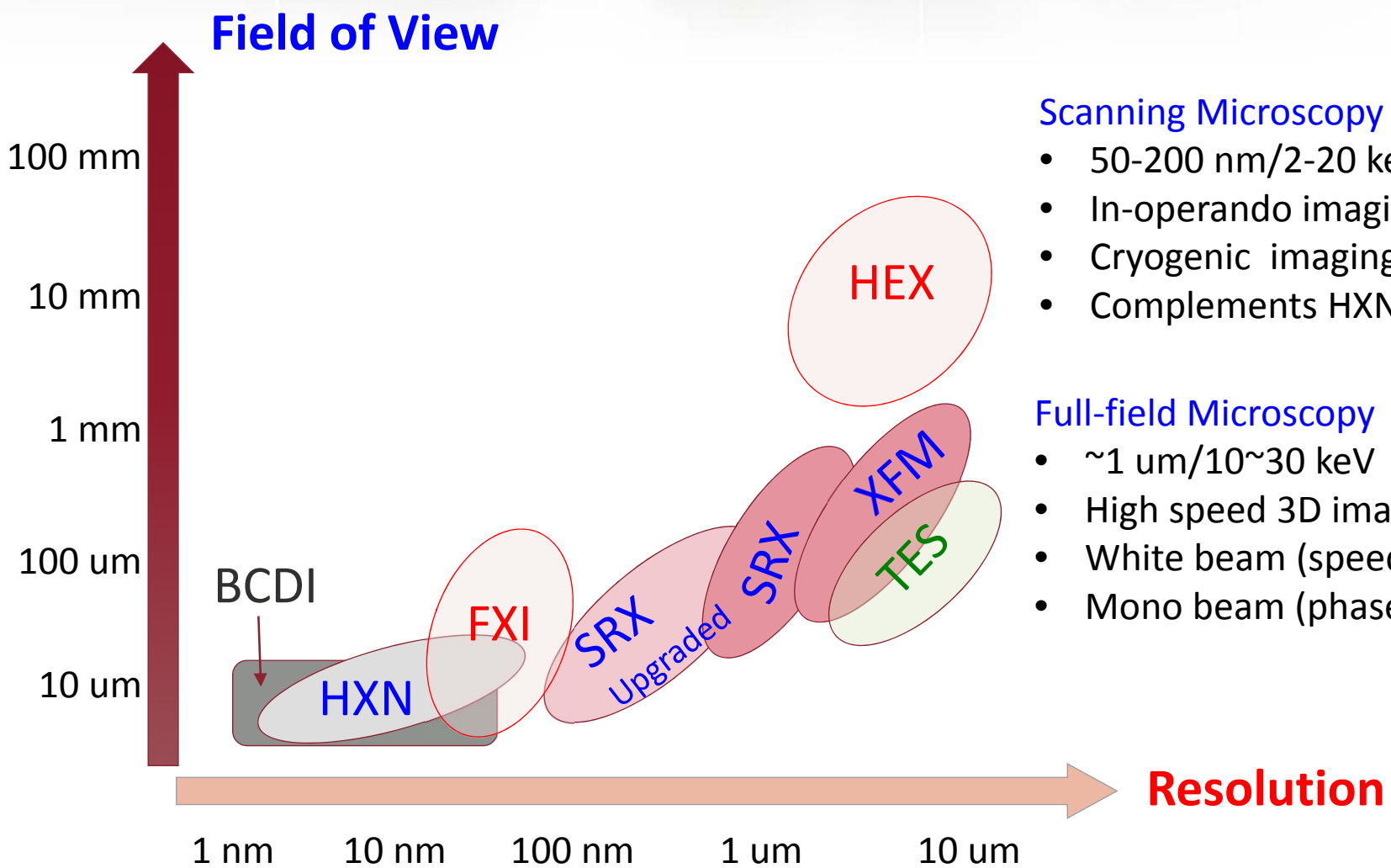
Imaging and Microscopy Program

- Program Description and Goals:
  - Develop and provide a suite of cutting-edge, multiscale, multimodal hard X-ray imaging and microscopy tools for wide range of scientific applications
- Hard X-ray Nanoprobe (HXN):
  - Upgrade endstation with interferometer-tracked rotation and wedged MLLs, and upgrade conditioning optics → total ~10x flux improvement
  - Upgrade of data acquisition controls to enable fly- scan speed upgrade to ~1 ms/pixel → 30x improvement



- Sub-um Resolution X-ray Spectroscopy (SRX):
  - Develop new KB microscope replacing old system with a broken mirror
  - Provide multimodal imaging (XRF, XRD, DPC, spectroscopy, tomography) with routine fly-scan capabilities and high positioning stability for 100 nm resolution
  - Developing confocal XRF capability in collaboration with Corenll
- Full-field X-ray Imaging (FXI), Tender Energy Spectroscopy (TES), and X-ray Fluorescence Microscopy (XFM):
  - All relatively new BLs, ramping up capabilities and corresponding user programs
  - Possible 2nd sample chamber at TES dedicated for catalysis research under discussion

Capabilities Gaps in Imaging & Microscopy



Scanning Microscopy

- 50-200 nm/2-20 keV
- In-operando imaging
- Cryogenic imaging
- Complements HXN/SRX

Full-field Microscopy

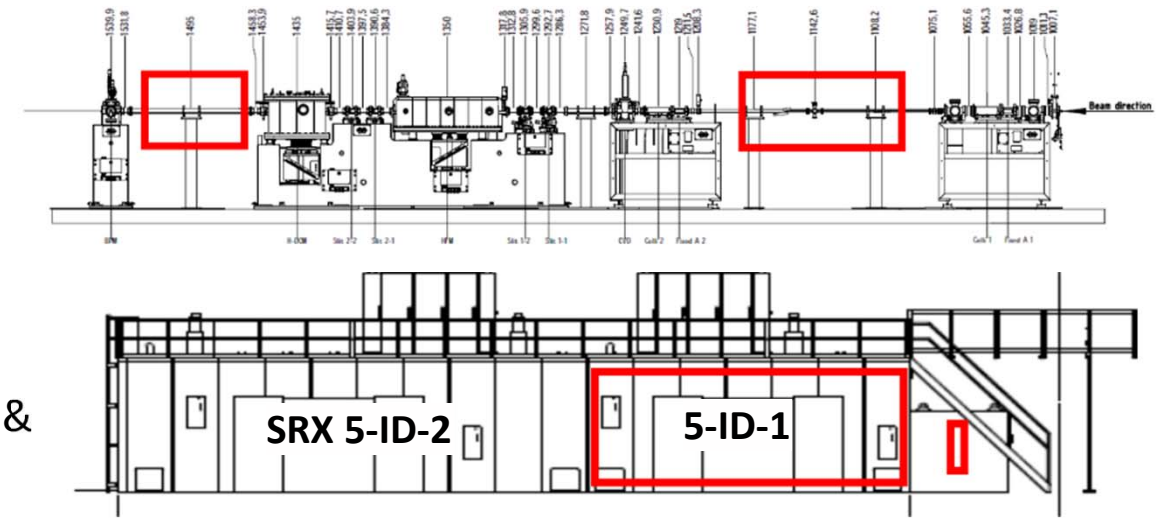
- ~1 um/10~30 keV
- High speed 3D imaging
- White beam (speed)
- Mono beam (phase-contrast)

Newly Proposed Imaging and Microscopy BLs

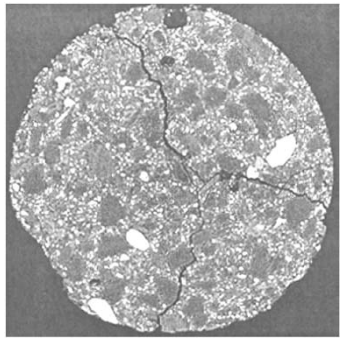
- In-situ Nanoprobe at 5-ID-1 (ION & CXN):
  - Leveraging infrastructure built-in at SRX side-branch (hutches, front-end, PPS)
  - Two endstations:

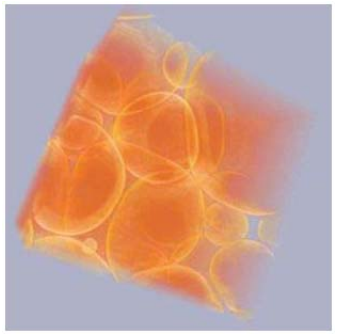
    ION - in-situ/in-operando nanoprobe at 50-200 nm

    CXN – cryo XRF nanoprobe for cryo imaging of biological & environmental applications

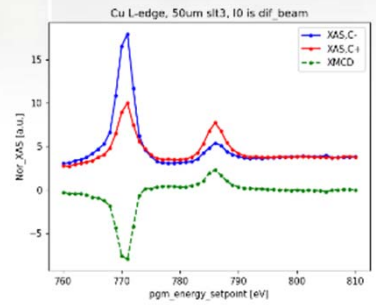


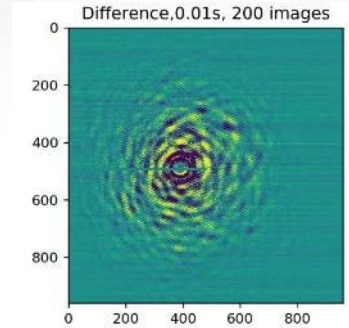
- Micro-CT Beamline (MCT):
  - Microtomography with white and mono beam options; E ~ 10-30 keV, on 3PW
  - High-speed imaging and phase-contrast
  - Wide-range of science applications – fatigue and cracks in materials, batteries, soils and plant seeds, insects, rock-fluid systems, ……





Soft X-ray Scattering & Spectroscopy





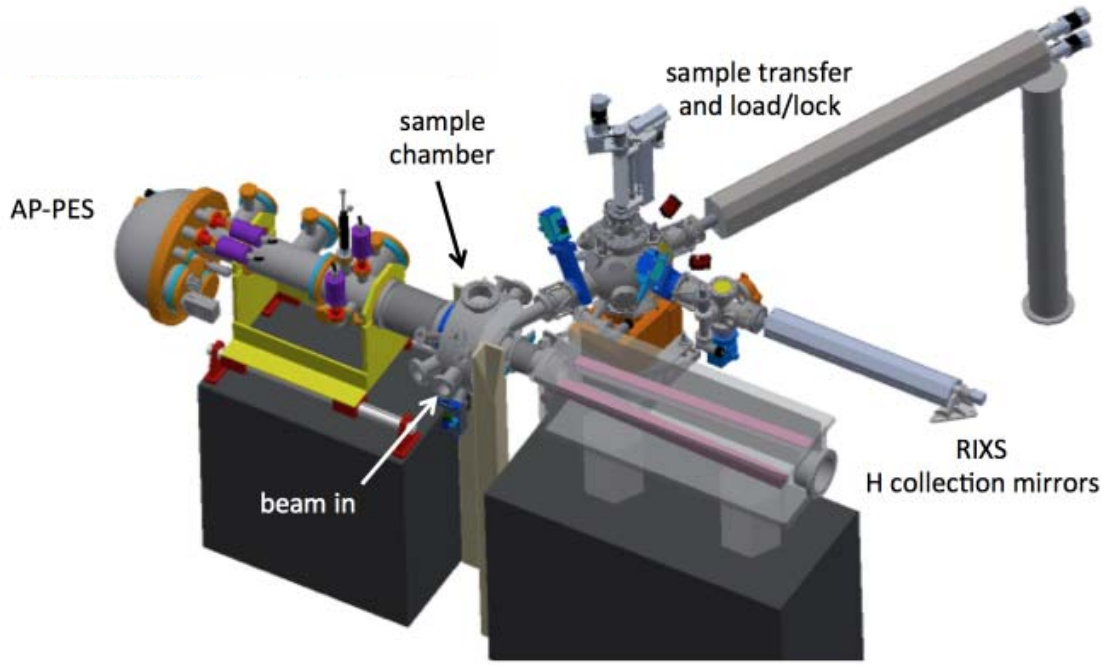
- Program Description and Goals:
  - Soft X-ray scattering & spectroscopy combined with imaging to enable science in quantum materials and catalysis & energy research
- Coherent Soft X-ray Scattering (CSX):
  - Continue to support XPCS on emergent heterogeneous condensed matter systems
  - Mature spatially resolved scattering capabilities at nm-scale, and develop holography for magnetic domain and skirmions imaging, in close coordination with I&M program
  - Finalize and implement revised canting plan to remove interference between CSX/IOS
- In-situ and Operando Spectroscopy (IOS):
  - Develop & implement an upgraded IO-XAS endstation
  - Develop a new multimodal endstation INSPIRE
  - Coordinate with hard X-ray programs for better synergies for catalysis research at NSLS-II
- Electron Spectro-Microscopy (ESM), Soft Inelastic X-ray Scattering (SIX), and Frontier Infrared Spectroscopy (FIS/MET):
  - Complete commissioning and ramp up user operations at ESM and SIX
  - Complete construction of FIS/MET and transition into operations

Gap Analysis in Soft X-ray Scattering & Spectros.

- For quantum materials move from 20th century science (big crystals) to 21st century materials which requires the understanding and control non-heterogeneity and the functioning of nanostructured devices
- Understanding these will require nanostructure determination of
  - Crystalline structure → Nanoprobe (HXN…)
  - Electronic order → REXS (CSX)
  - Electronic structure → ARPES (ESM)
  - Electronic Excitations → RIXS (SIX), IR (MET)
- Current research needs are pushing into the imaging regime → new capabilities:
  - ARPES/RIXS imaging of electronic inhomogeneities at nanoscale resolution → ARI
  - STXM to provide much needed imaging capabilities in the soft region to obtain contrast for quantum materials, energy science, and soft matter → SMF
  - Near-field (IR) spectroscopy at very high spatial resolution (nm) → INF
  - Opportunity to combine RIXS and AP-PES into a novel instrument → INSPIRE = QIX/AP-XPS/IRRAS
  - Multimodal access combining electronic and structural imaging
  - Tender x-ray inelastic scattering (TIN) that complements SIX

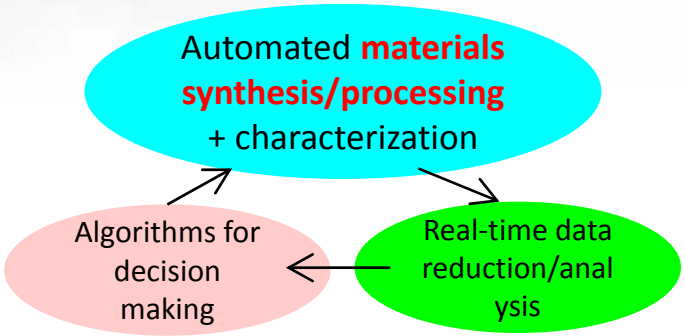
New INSPIRE Endstation at IOS

- INSPIRE (INelastic Scattering, Photoemission, and InfraRed Endstation)
  - Concept evolved from QIX (Quick Inelastic X-ray Scattering) from the 2016 beamline development proposal process
  - New endstation INSPIRE and optics upgrades to the IOS (23-ID-2) beamline that will enable ambient pressure XPS, XAS, IR, and XES/RIXS experiments on the same system under the same close-to-realistic operating conditions
- Science areas:
  - Catalysis: Reveal the kinetics of catalytic reactions
  - Materials Science: Track changes in electronic structure and surface composition
  - Batteries: Unravel multisc processes and dynamics under working conditions



Complex Scattering Program

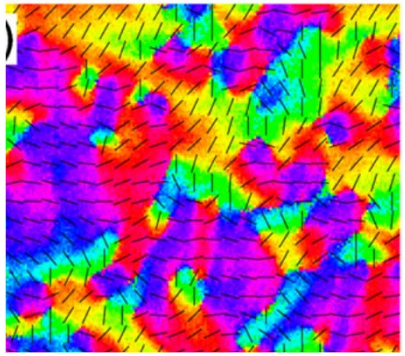
- Program Description and Goals:
  - Provide a suite of X-ray scattering tools address grand scientific challenges relevant to soft matter
  - AI guided parameter mapping to optimize structure-function and non-equilibrium properties during synthesis, processing, as well as in operating devices



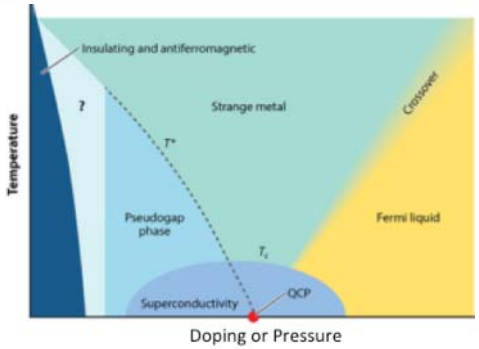
- Coherent Hard X-ray Scattering (CHX):
  - Continue to develop XPCS methods and analysis for the studies of interplay between macroscopic properties and nanoscale dynamics in complex systems
  - Implement novel VIPIC detector to push the boundaries of XPCS with 20ns time stamps
  - Coordinate with APS and develop a common library of analysis software tools
- Inelastic X-ray Scattering (IXS):
  - Complete optics optimization for 2-meV to improve counting efficiency by up to 10x and explore single reflection collimating optics to enhance analyzer efficiency
  - Develop long-term plans for improved source, optics, and parallel data acquisition
- Complex Materials Scattering (CMS), and Soft Matter Interface (SMI):
  - Continue to ramp up user programs and deliver as designed capabilities
  - Complete detector upgrade; continue to develop autonomous experiments/analysis
  - Complete J-PLS and establish liquid scattering & polymer processing capability at SMI

Newly Proposed BLs in Complex Scattering

- Soft X-ray STXM for Soft Materials (STX):
  - Key scientific directions of soft matter & organic devices: chemical & orientational domains, regenerative bio-tissue and cells, ionic distributions in water filtration membranes
  - Complements the RSoXS and NEXAFS capabilities on SST. Will include cryo capability for bio-synthesis/printing applications
  - STX would be on a BM or 3PW beamline, or could be a branch on a 3PW beamline

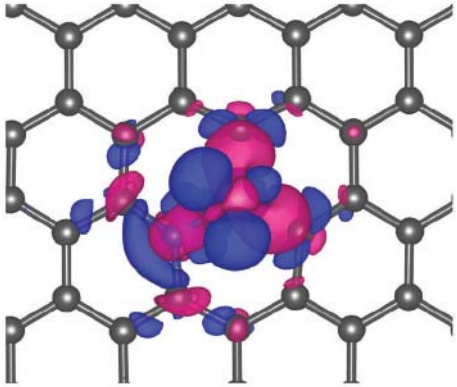


- Tender and hard x-ray Inelastic scattering Nanoprobe (TIN):
  - World's first X-ray nanoprobe of electronic excitations using resonant/non-resonant IXS in the tender (2.5 – 4 keV) and hard (5 – 15 KeV) ranges with 50-nm spatial resolution and tunable energy resolution up to sub-10 meV
  - Science case examples:
    - Nanoscale ordering in QIS materials such as superconducting Weyl semimetals, spin liquids, topological superconductors, spin textures
    - Imaging of charge dynamics in catalysis and energy storage materials under operando conditions
    - Novel materials dynamics and quantum phase transitions under high pressure



Hard X-ray Spectroscopy Program

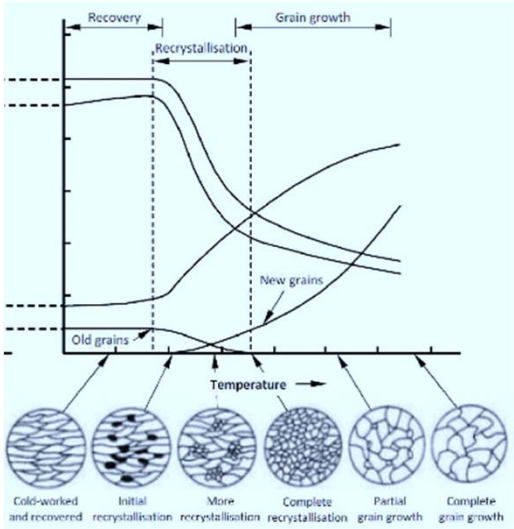
- Program Description and Goals:
  - Provide a suite of world-class high-throughput operando X-ray spectroscopy tools, coupled with advanced modelling and materials databases to enable visualizations of atomic-scale structures in real chemical processes
  - To understand structure-function correlations and allow development of better synthesis of advanced catalysts and functional materials



- Inner Shell Spectroscopy Beamline (ISS):
  - Develop high-throughput reaction environments to take advantage of high X-ray flux
  - Seamless integration of operando infrastructure (potentiostats, mass-flow controllers etc) into beamline controls system
  - Develop batch mode user access to combine multiple user groups in a single run
  - Develop sample database-driven data acquisition and analysis pipeline
- Quick Absorption and Scattering (QAS), NIST Beamlines (SST-1, SST-2, BMM):
  - Complete commissioning activities and ramp up user operations
  - Develop better synergies between soft and hard X-ray spectroscopy techniques

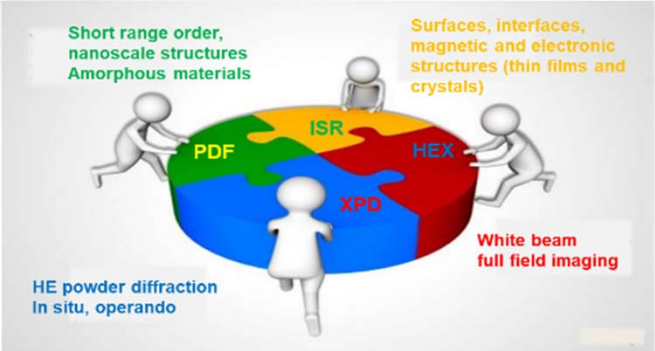
Newly Proposed BLs in Hard X-ray Spectroscopy

- Catalysis & Growth Village (CGV):
  - A combination of high throughput **soft** and **tender** X-ray Absorption (focused on in-situ/operando) stations, a set of 3 (or more) ambient pressure XPS chambers (including High Energy XPS) dedicated to "dirty chemistry", and a soft X-ray resonant coherent scattering chamber dedicated to operando and in-situ experiments
  - A full sector for CGV: BM for high-throughput XAS and AP-XPS, and ID beamline for a canted tender and soft X-ray with full polarization control, with multiple endstations; Could also accommodate INSPIRE endstation; Potentially a large user community
  - Take full advantage of the synergy with data and theory effort within the Program
- Additive Manufacturing Scattering facility (AMS):
  - A high-energy diffraction facility (on HEX-2 or HEX-3) for certification process in additive manufacturing of metal alloys, in partnership with AFRL & industry
  - Focus on strain/stress and crystallite size & orientation determination of defined sample geometries
  - Competitive advantage with a dedicated setup with fully integrated and automated data pipeline infrastructure compatible to NIST data basis



Diffraction & In-situ Scattering Program

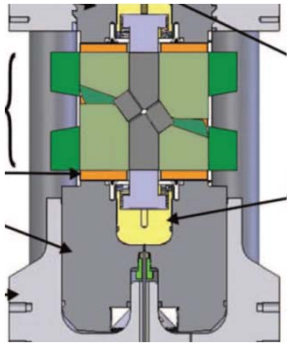
- Program Description and Goals:
  - Provide world-class capabilities in X-ray powder and single-crystal diffraction for studying complex, heterogeneous, and disordered materials under in-situ and operando conditions



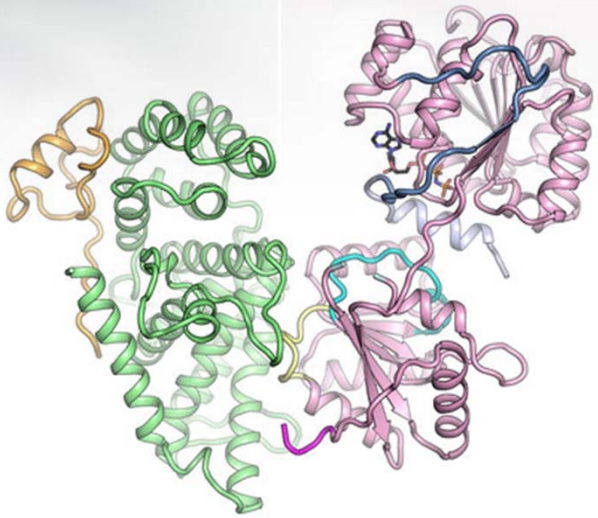
- X-ray Powder Diffraction (XPD):
  - Continue to serve a large user community; Identify and focus on areas of excellence in science program; Maintain high productivity with automated measurements
  - Commission multi-anvil setup for high-pressure research in partnership with COMPRES
  - Develop and commission X-ray diffraction tomography in Hutch D
- X-ray Pair Distribution Function (PDF):
  - Complete commissioning and ramp up user programs
- In-Situ Resonant Scattering (ISR):
  - Continue to ramp up user science programs and additional as-designed capabilities
  - Commission tender X-ray capability for studies of 4d transition metal compounds
  - Develop sub-100nm micro-diffraction capability using kinoform lenses
  - Develop a versatile LN2-free magnet and phase-plate for studies of magnetic materials

Newly Proposed BLs in Diffraction Program

- Multi-dimensional Multi-modal Diffraction (MMD):
  - Strengthen NSLS-II diffraction capabilities by enabling extended diffraction mapping and imaging with a tunable X-ray focus down to ~100 nm, with two endstations
  - Micro-diffraction to probe changes in atomic and nanoparticle structures, defects, and inhomogeneities during synthesis reactions, phase transitions, or device operation
  - High-flux, high-angle resolution, high-throughput powder diffraction or diffuse scattering on single crystal diffraction
- Coherent In-situ and Operando Studies of Materials (CSO or ISR-2):
  - In-situ coherent scattering studies of growing thin-films and nano-materials and material synthesis, enabling Co-GISAXS, XPCS, and imaging techniques
  - Science applications in new functional materials such as monolayers on substrates (Graphene, WSe_2) or as nano-particle/substrate that are best studied in situ or operando
- Multi-modal High Pressure Tools (MPT):
  - ED-/AD-XRD at HEX-2 or HEX-3 for studies of 3D distribution of strain and structure as a function of pressure, temperature, and time in order to model mechanical, thermodynamic, and kinetic properties
  - Science applications in energy (fracking, carbon sequestration), water in subsurface, earth science, and materials synthesis



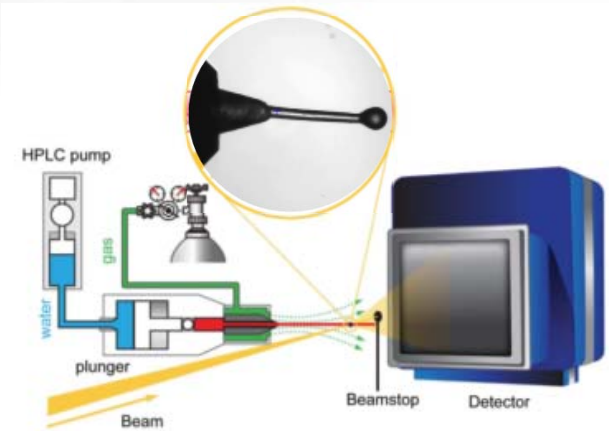
Structural Biology Program



- Program Description and Goals:
  - Provide world-leading capabilities in MX and X-ray scattering to enable discovery-class research on fundamental biological questions
  - Scientific focus is to investigate the molecular structure and function of complex biomolecules using extremely small crystals and molecules in solution
- Frontier and Automated Macromolecular Crystallography (FMX, AMX):
  - Continue to ramp up user programs and produce impactful research results
  - Develop serial MX methods with crystal delivery techniques and highly merged datasets
  - Develop & implement biochemistry methods for studies of kinetics in biomolecules
  - Develop a multilayer monochromator for FMX to enable time-resolved serial MX
- Life Science X-ray Scattering (LiX), X-ray Footprinting (XFP), NY State MX (NYX):
  - Continue to ramp up user programs at LiX and XFP
  - Mature partnership with SNS/HFIR for coordinated access of both SANS and SAXS at LiX
  - Complete installation and commissioning of Bio-XAS endstation at XFP
  - Complete commissioning of NYX and start to ramp up user program

Newly Proposed BLs in Structural Biology

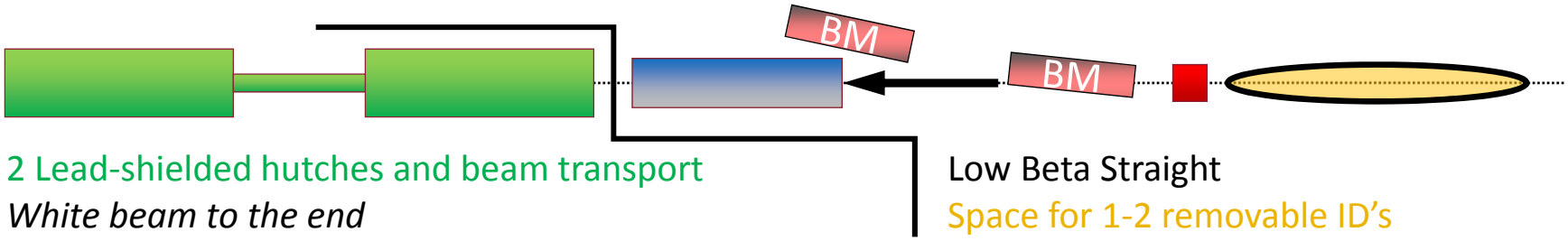
- High-flux Serial Micro-crystallography (HSX):
  - Dedicated world-class Serial Micro-crystallography beamline with a high-flux multilayer monochromator
  - A suite of crystal delivery methods (LCP injection, acoustic droplet, in-situ crystallization plates, etc.) to make serial MX routine at room temperature
  - Automated data processing capable of merging large numbers of datasets from thousands of crystals



- Fixed Energy MX (FEX):
  - Two fixed-wavelength beamlines for MX viewing an undulator source, leaving space in the sector to accommodate a second (canted) undulator and tunable BL built later
  - Opportunity exists to deliver substantially higher MX beamline capacity than currently exists at NSLS-II. With the proposed beamlines, NSLS-II could support ~500,000 samples/yr and attract new communities including those displaced elsewhere
  - Ideal for MX experiments for which wavelength tunability isn't vital – reducing load on AMX, FMX, and NYX, allowing them to focus on their unique capabilities
- Massively Automated MX (MAX):
  - Extreme-level automation at this MX facility would accommodate mail-in samples only
  - Built upon intelligent robotics and DAQ, and autonomous data processing

New Metrology and Test Beamline (MTB)

- Test beamlines have seeded many significant developments: refractive optics, phase contrast imaging, wavefront sensing, inelastic scattering instrumentation, UHRES monochromators, x-ray polarizers and undulators
- Metrology and Test Beamline (MTB):
  - A flexible beamline located on a straight section to serve as a test platform for IDs, X-ray optics, detectors, instrumentation and techniques
  - Unique capability to NSLS-II and DOE complex (open straight section, white beam and flexible optics), complementing development efforts in all beamline programs
  - Supports long-term collaborations on detector and other instrumentation development
  - Can an ideal home to the MCT endstation with potential of high productivity



2 Lead-shielded hutches and beam transport

White beam to the end

Movable components:

- *Monochromator, Detector test station*
- *Focusing mirror, 4-circle goniometer*
- *Metrology test station*

Low Beta Straight

Space for 1-2 removable ID's

3-pole wiggler at downstream end

3PW and ID-compatible front end

Transfocator in the front end

Summary of New Beamlines Concepts

New Beamlines: already approved & newly proposed		
Soft X-ray Scattering & Spectroscopy	ARI	ARPES and RIXS Nano-Imaging
	QIX/INSPIRE	RIXS/XES, Photemission, and Infra-Red Endstation
	SMF	Soft X-ray STXM Spectro-Microscopy Facility
	INF	Infrared Near Field Nanospectroscopy for Interface Technology and Emergence
Diffraction & In-Situ Scattering	MMD	Mutlidimensional Multimodal Diffraction
	ISR2	Integrated In-situ and Resonant Hard X-ray Studies 2
	MRE	Materials in a Radiation Environment
	MPT	Mutlimodal High Pressure Tools
Image & Microscopy	CDI	Coherent Driffraction Imaging
	MCT	Micro Computed Tomography
	ION/CXN	In-situ and Operando Nanoprobe / Cryo X-ray Nanoprobe
Expt'l Dev.	MTB	Metrology and Test Beamline (possibly equipped with MCT endstation)
Hard X-ray Spectroscopy	CGV	Catalysis and Growth Village (soft and tender X-rays)
	AMS	Additive Manufacturing Scattering Facility (hard X-rays)
Complex Scattering	PLS	Processing and Liquid Surfaces
	STX	Soft X-ray STXM for Soft Materials
	TIN	Tender and Hard x-ray Inelastic scattering Nanoprobe
Structural Biology	MAX	Massively Automated Crystallography
	HSX	High-flux Serial Crystallography
	FEM	Fixed Energy MX
	LAX	Long-wavelength Automated Crystallography

Thanks to Ignace Jarrige and Juergen Thieme for coordinating activities

Review of New BL Concepts and Next Steps

- We have reviewed all new BL concepts, with the following initial assessments:
  - Almost all new beamline concepts identified the existing capabilities gaps in our current portfolio at NSLS-II
  - A number of proposed BL concepts are much more mature than others, particularly on their science cases, while other concepts require more work on targeted research areas and/or technical implementations
- Proposed path forward:
  - Continue to engage program staff to sharpen the science cased and technical schemes
  - Start to discuss potential funding for those beamline concepts that are better defined, and iterate with stakeholders
  - Plan to hold an all-day Strategic Planning Workshop at the annual Users Meeting in May 2019 to engage the broad community for further input and dialog
  - Continue to involve SAC in this process

Strawman Development Scenarios of New BLs

- DOE-BES major items of equipment (MIE) project:
  - CDI: Bragg-CDI for world-class lensless imaging down to 5 nm
  - SMF: Soft x-ray STXM with nm-scale resolution via ptychography
  - INF: Nano-IR spectroscopy of heterogeneous solid state materials
- DOE-BES SUF/ADR:
  - MTB: Metrology and test beamline, with micro-CT (MCT) endstation
- Expanded BDN portfolio:
  - QIX → INSPIRE: multi-modal studies of snapshots of chemical reactions in-operando
  - ION: in-situ operando nanoprobe, with BER-funded cryo-XRF nanoprobe 2nd endstation
- Other possible funding:
  - ARI: simultaneous nano-APPES/nano-RIXS at ~100 nm resolution → NSF for endstation
  - PLS/STX: polymer & liquid processing / bio-printing → DOE-BES, DoD/DoC, NSF ?
  - CXN: cryo XRF nanoprobe → DOE-BER
  - AMS (HEX-2): DoD + industry ?
  - MPT (HEX-3): NSF/COMPRES ?
  - HSX/FEX/MAX: NIH ?

Summary

- New NSLS-II Strategic Plan 2019-2023 being developed; It will outline major development activities for next five years
- With the DOE MIE CD-0 proposal being launched, we are starting to conceptualize a plan to buildout additional beamlines at NSLS-II
- We have solicited new beamline ideas and concepts from staff, and will engage the scientific community in the coming months to further develop these concepts
- Any feedback from SAC on these beamline concepts as well as on our strawman plan how to best fund these new beamlines, are welcome and appreciated