Vision for the Future

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Triennial Operations Peer Review

June 20-21, 2017

Outline

- Planning process
- Overview of 2017 strategic plan
- Facility improvement plans in next five years
- Beyond next five-years
- Summary

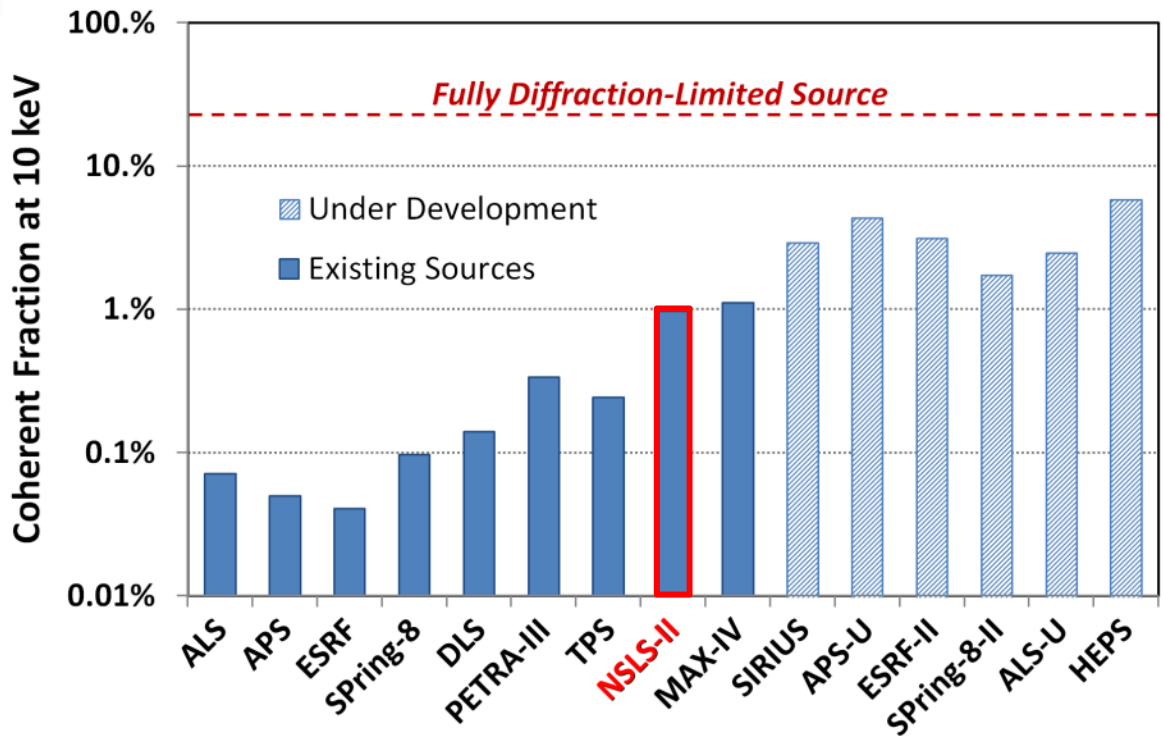
https://www.bnl.gov/ps/docs/pdf/NSLS2-Strategic-Plan.pdf

Community Fully Engaged in Strategic Planning Process

- Starts with discussions with scientific user community to identify strategic science directions and required NSLS-II capabilities
- Integrates community input in construction and operations – SAC, UEC, BATs, topical workshops, reviews, ……
- Previous NSLS-II strategic planning focused on new beamlines selections and early science
- This round of strategic planning:
  - evolving from mostly construction to operating
  - competing priorities with challenging fiscal outlook
- Goals for *2017 Strategic Plan*: high-level strategic plan *and* actionable plan to serve as basis for budget priorities for all major activities

NSLS-II Has a Competitive Advantage Now

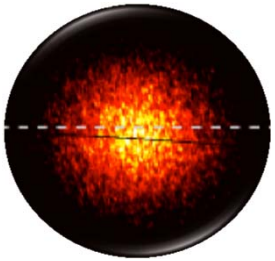
- In the next five years, we will play a transformative role in:
  - science in coherence & nano-imaging to tackle grand challenges
  - innovative user modes to maximize scientific impact of NSLS-II
  - advancing high-brightness technologies in coherence and nano-focusing



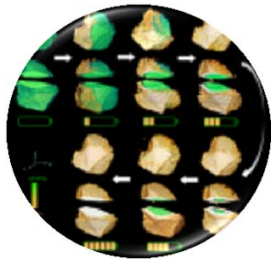
- Excellent opportunity to work together with other facilities in support of DOE-BES scientific user facilities mission

NSLS-II Strategic Scientific Directions

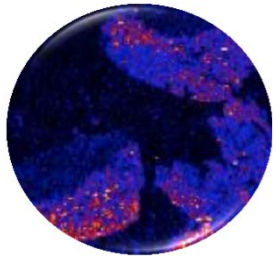
- Emergent Behavior and Complexity:
  - Complexity and dynamics of emergent interacting phases and intrinsically heterogeneous systems
  - NSLS-II: coherence, nano-imaging, & inelastic scattering ideal for studies of heterogeneities & naturally-occurring dynamics



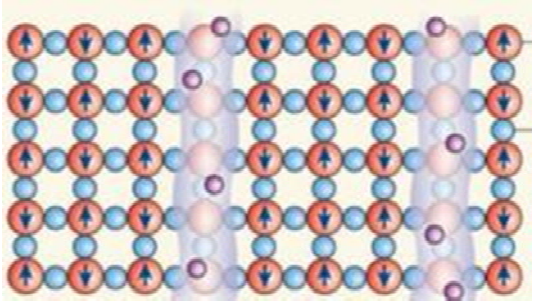
- *In-situ* and *Operando* Science:
  - Understandings of how things work in functioning environment and under working conditions in actual devices & systems
  - NSLS-II: high flux in broad spectral range for *in-situ* and *operando* studies of functional systems



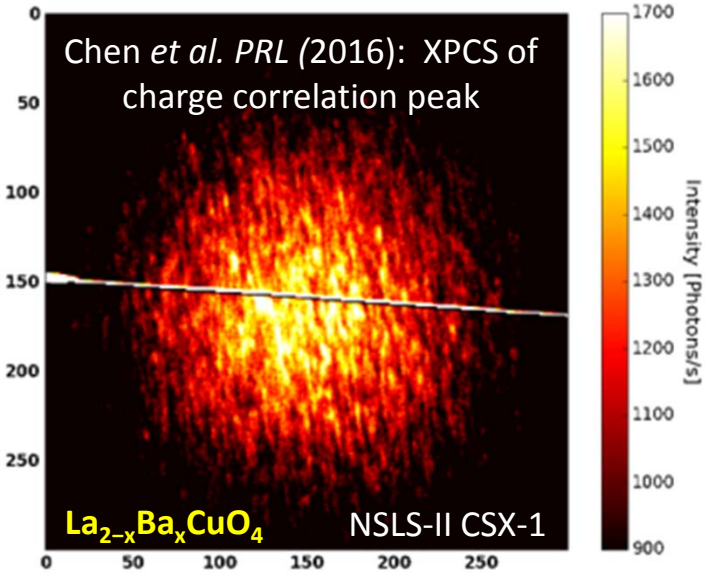
- Multiscale Structures and Functions:
  - Structural, electronic, and chemical behavior on length and time scales between atomic and macroscopic world
  - NSLS-II: suite of imaging tools for structural, chemical, & electronic imaging across multiple spatial and temporal scales



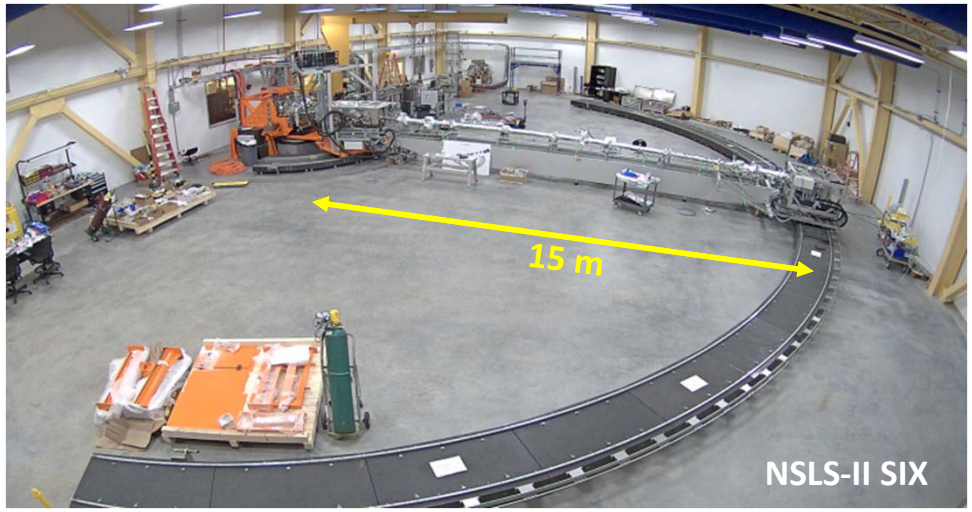
Science Vision 1: Imaging Stripes Dynamics in High-Tc Cuprate



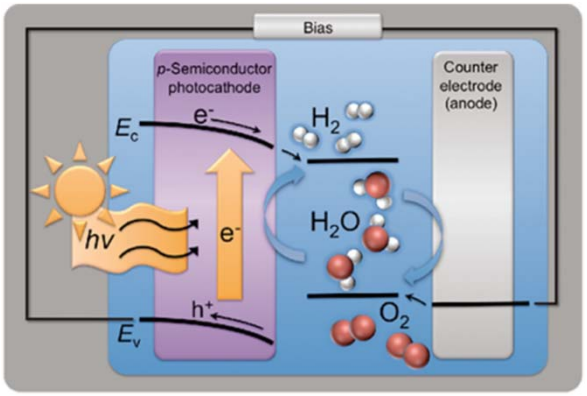
Tranquada (1995)

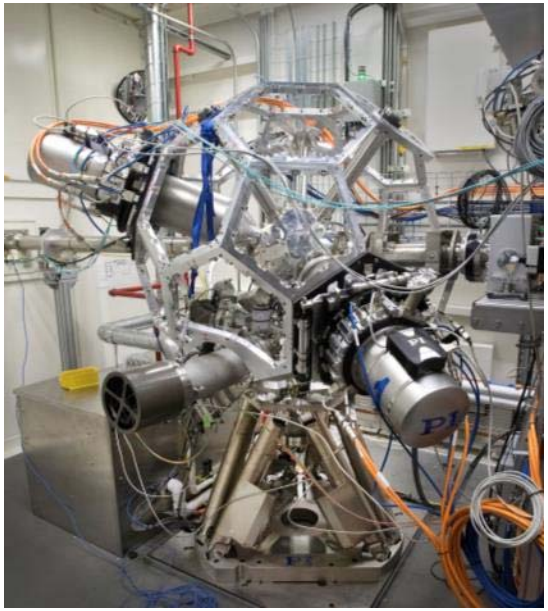


- High coherence at NSLS-II enabled **first ever** speckle and XPCS measurement of charge stripes in a cuprate at CSX-1
  - Stripe correlations found to be static
- Role of stripes in spin fluctuations still unknown
  - Will be investigated using soft x-ray RIXS at SIX at world-leading 15 meV resolution

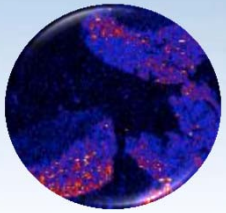


Science Vision 2: Accelerate Materials Design in Water-Splitting Process



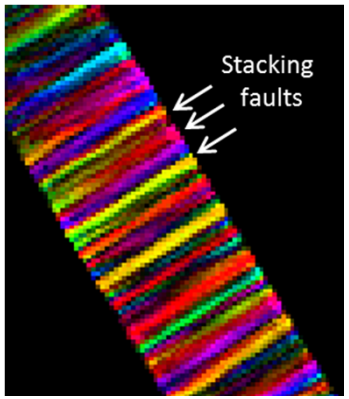


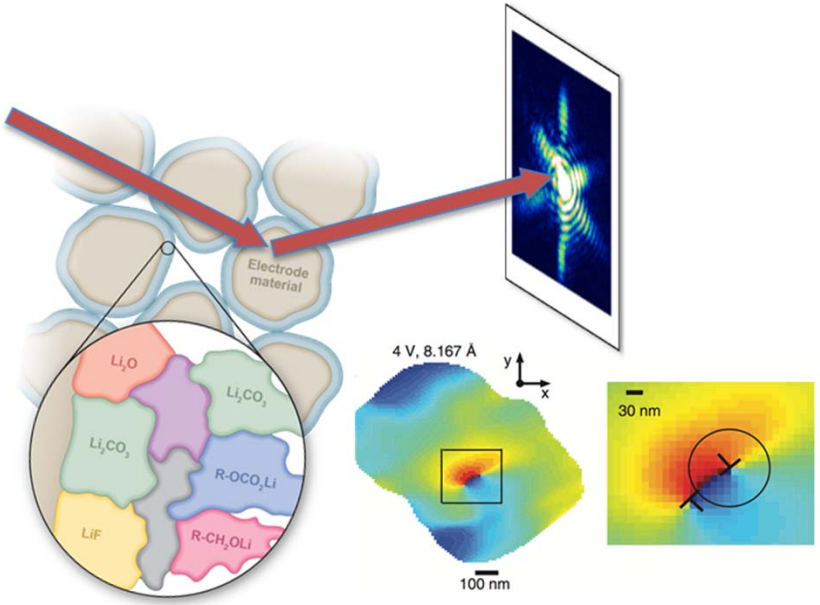
- Water-splitting systems require very efficient photocathode and catalyst to speed up the chemical reaction that splits water into hydrogen and oxygen
- Much research being done to optimize the photocathode design and synthesis but require many iterations in design-synthesis-testing cycle
- In-situ/operando studies at NSLS-II ISS beamline with gas-handling will dramatically speed up this process:
  - Photocathode synthesis reactor with in-situ XRD & XES monitoring for structure & electronic states
  - In-situ/operando XAS/XES studies of cathode performance during water-splitting reaction
  - Allowing researchers to design, fabricate, and characterize materials and their function in just a few experiments



Science Vision 3: Imaging of Electrode Grains and Interfaces in a Li Battery

- Bragg ptychography at HXN and CDI beamlines will enable routine multi-grain strain mapping of polycrystalline materials structures and correlate with their performance
- Potentially high impact experiment would be to investigate how a Li battery electrode degrades following charge and discharge cycles
  - multi-grain structures and their interfaces
  - strain fields and defects within single grain
  - under operando or in-situ conditions



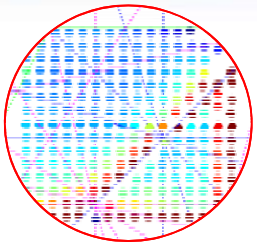


Imaging Li battery electrode to see how it changes and degrades following Li insertion and deinsertion

Beamline Programs Aligned with NSLS-II Strategic Directions to Address Scientific Challenges

	NSLS-II Beamlines	CSX-1	CSX-2	ESM	SIX	FIS	MET	ISS	TES	QAS	SST-1/-2	BMM	IXS	CHX	CMS	SMI	XPD	PDF	ISR	HEX	HXN	SRX	XFM	FXI	LIX	FMX	AMX	XFP/XAS	NYX
NSLS-II Science Themes	Emergent properties & complexity	■	■	■	■		■				■		■	■	■	■			■		■	■	■	■					
	In-situ and operando science		■			■	■	■	■	■		■			■	■	■	■	■	■	■	■	■	■	■			■	
	Multiscale structure & function	■		■		■			■		■			■			■			■	■	■	■	■	■	■	■	■	■
Grand Challenges in Basic Energy Sciences	Processes at the levels of electrons	■	■	■	■			■	■	■	■	■							■										
	Synthesis for tailored functions			■				■				■			■	■	■	■	■										
	Control of emergent properties	■	■	■	■	■	■					■			■	■			■	■	■	■	■						
	Energy & information on nanoscale	■		■							■			■				■			■	■		■	■			■	
	Systems away from equillibrium	■					■						■	■	■	■			■	■				■	■				
Grand Challenges in Bio-Environmental Sciences	Genome to microbial & eco-systems								■													■	■						
	Earth's subsurface environment					■			■								■			■		■	■	■					
	Physics and chemistry of life												■	■	■	■								■	■	■	■	■	■
	How cells work with environment								■												■	■	■	■	■	■	■	■	■
	Molecular basis of bio-diversity																			■				■	■	■	■	■	■

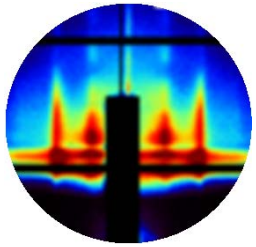
Crosscutting Enabling Technologies



- Accelerator Science and Technology:
  - *Develop effective technologies for stable and reliable operations and for enhancing the performance of NSLS-II accelerator complex*

- Advanced X-ray Technology:
  - *Develop innovative technologies in nanofocusing & coherent x-ray optics, experiment simulations, and advanced pixel-array detectors*

- Multimodal Sample Environments:
  - *Taskforce formed to develop and implement strategies to enable and promote multimodal studies from in-situ/operando energy and materials sciences to multiscale bio-environmental research*



- Data Science and Computing:
  - *New DAMA group formed to develop and execute plans to provide advanced DAQ and analysis tools to enhance productivity & impact*

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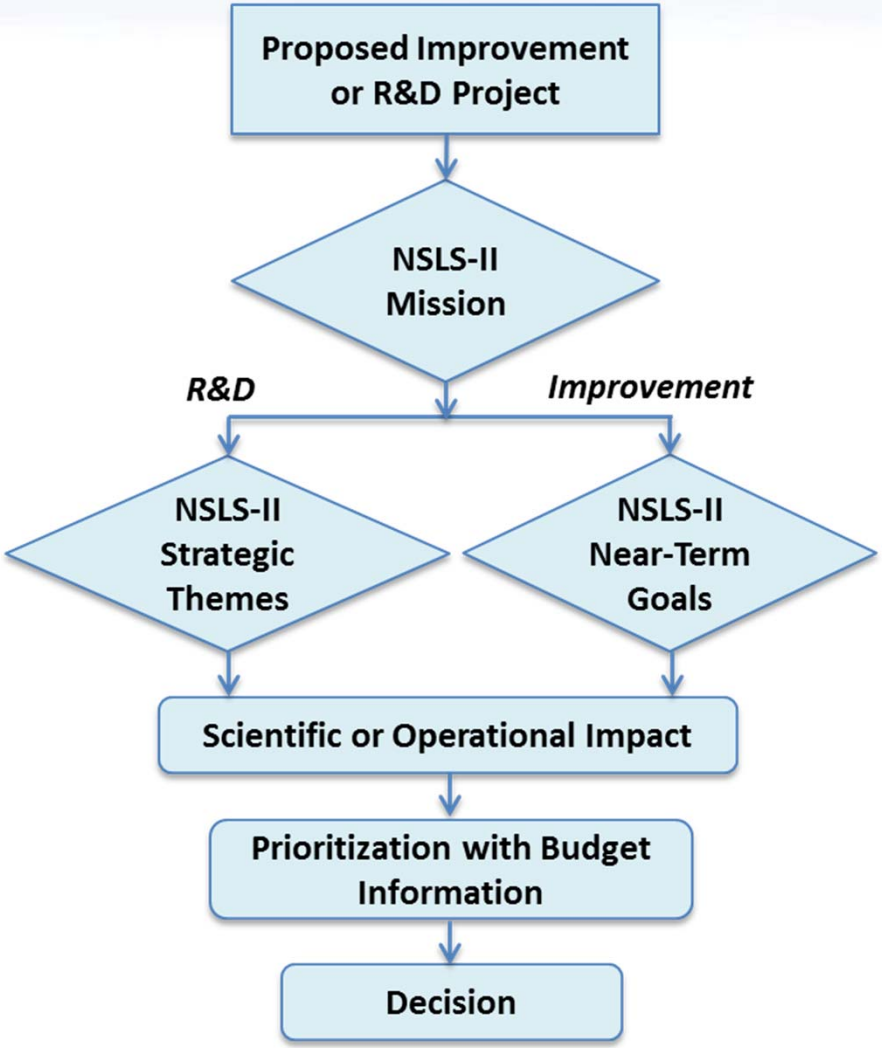
Prioritization and Selection Process

- NSLS-II uses an effective selection process (illustrated at right) at the division and the facility levels to prioritize major improvement and development activities and make decisions
- To-date majority of investments heavily weighted towards new beamline development
- Going forward we plan to increase the level of investments on existing beamlines and accelerator systems



R&D Example: LDRD Project Selection

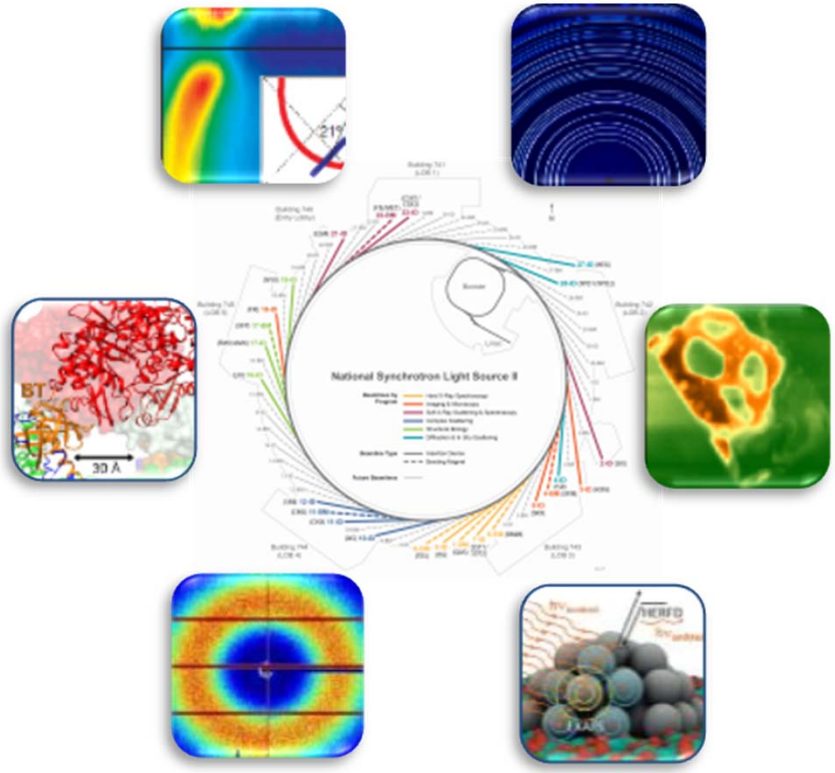
LDRD	Description	PI	Actual FY15 ($k)	Actual FY16 ($k)	Expected FY17 ($k)	Strategy
12-018	Conical Slit for Probing Buried Micron or Sub-Micron Volumes for Dynamic Measurements	N. Bouet	15.9	0.0	0.0	b
12-023	Femto-second X-ray Pulse Generation by Electron Beam Slicing	L. Yu	31.3	0.0	0.0	a
13-031	Modulation Enhanced Diffraction: a new tool for powder diffraction and total scattering	E. Dooryhee	138.9	3.6	0.0	1
13-032	Development of At-Wavlgnth Metrology Tools	M. Idir	268.0	24.9	0.0	b
13-033	Multi Dim Imaging Data Analysis	W. Lee	283.3	28.2	0.0	d
13-034	Atomic resolution Element Map	E. Nazaretski	169.9	8.7	0.0	b
14-021	In-Situ Investigation of the Strain Distribtuion in Next-Generation 3D Transistors by Nano-XRD	H. Yan	181.3	100.1	0.0	2
15-038	Segmented Adaptive-Gap Undulator for High Flux and Brightness Hard X-rays at NSLS-II	O. Tchoubar &	340.8	365.9	0.0	a
15-031	IXS determination of the inter- and intra-particle dynamics of nanoparticle superlattices	A. Cunsolo	78.5	151.6	52.6	1
15-037	In-situ microscopy investigation of complex manganese oxides for energy storage	Y. Chu	250.0	216.1	97.7	2
15-034	Searching and sorting haystacks	S. McSweeney	53.1	210.7	133.6	3
16-006	Serial Micro Crystallography at Full Flux	M. Fuchs	0.0	139.3	156.0	3
16-007	3D Ptychography imaging without rotation using highly convergent X-ray beam	X. Huang	0.0	110.2	197.4	b
16-010	100fs single-shot electron beam slicing technology towards ultra-fast imaging	L. Yu, Y. Zhu, T.	0.0	352.0	332.0	a
17-015	NSLS II High Brightness Studies	E. Blum	0.0	0.0	276.0	a
17-016	Diffraction limited and wavefront preserving reflective optics development	M. Idir	0.0	0.0	189.0	b
17-017	Development of compact, high efficiency nanofocusing optics for hard x-ray nano-imaging	E. Nazaretski	0.0	0.0	94.6	b
	Total LDRD and PD		**1,811.0**	**1,711.3**	**1,528.9**	

- LDRD evaluated and selected based on NSLS-II strategic science and crosscutting technology directions

1. Emergent properties & Complexity	a. Accelerator science & technology
2. In-situ & operando studies	b. Advanced X-ray technologies
3. Multiscale structure & function	c. Multimodal sample environment
	d. Data-driven science

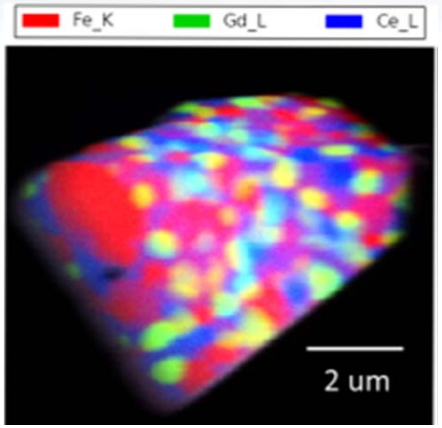
Accelerator and Beamlines Improvements

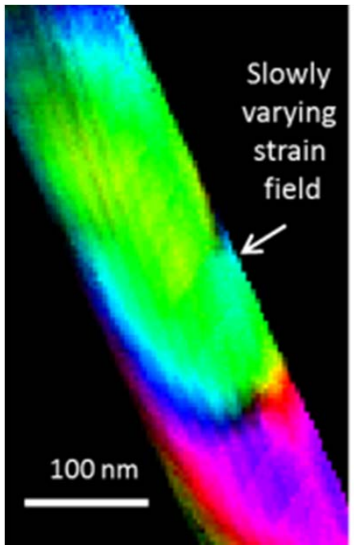
- Accelerator improvements priorities:
  - Baseline projects to **fix** known issues, optimize performance of subsystems
  - Improvements that significantly **improve** ops performance, increase beam stability and availability, and decrease downtime
  - R&D projects aimed at novel techniques for **upgrades** in the longer-term
- Beamline programs priorities:
  - Development of impactful **user science** programs at operating beamlines
  - Delivery of **new beamlines** currently under construction
  - Plans to **improve performance** and efficiency to accommodate more users
  - Optimizing output and **enhancing capabilities** to deliver more high-impact science



Beamline Example : HXN Beamline Plans

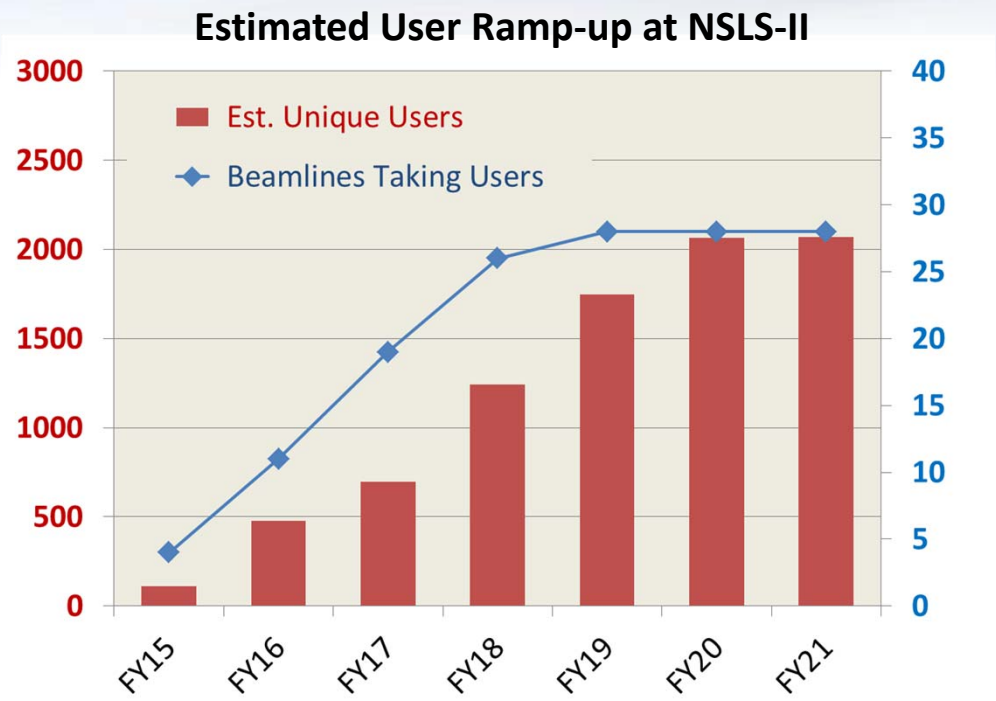
- GU operation authorized on Nov 9, 2015
- In FY17, main focus is on user science operations:
  - optimize user operations on 2D XRF imaging using MLL/ZP microscope
  - enhance visualization and analysis of multi-modality imaging – elemental imaging (XRF) & nanoscale morphology (DPC, ptychography)
  - enhance robustness of 3D XRF tomography.
- In FY18, mature user operations and offer add'l capabilities:
  - optimize 3D XRF imaging capability using the MLL microscope
  - provide a ptychography capability for GU with sub-5 nm resolution
  - optimize in-situ experiments using electrochemical controls (battery, corrosion) and current/voltage measurements (solar cells, etc.)
  - expand Bragg ptychography capability for quantifying strain distribution within single crystal grains.
- In FY19-21, pursue enhanced capabilities:
  - streamline all on-line analysis tools, so that even non-experts can perform experiments without difficulties
  - enable variable sample temperature controls (from ~90K to ~900K)
  - work with optics group to improve MLL optics with a goal to deliver sub-10 nm focus





User Program

- We will see a rapid increase in number of users in next five years
- We will enhance user access modes and efficiency in
  - Mail-in and remote
  - Multimodal and multi-beamlines
  - Joint proposals with other user facilities (CFN, SNS/HFIR, CSI, …)

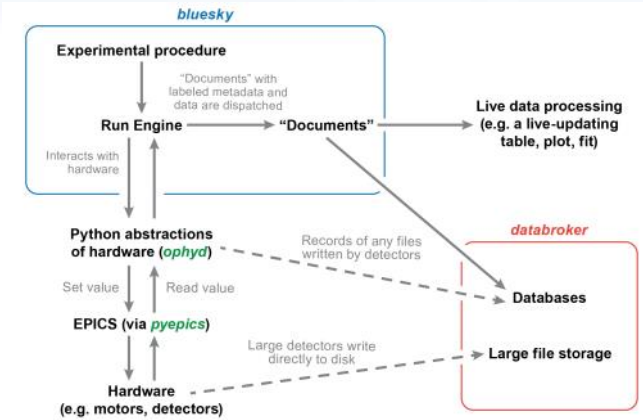


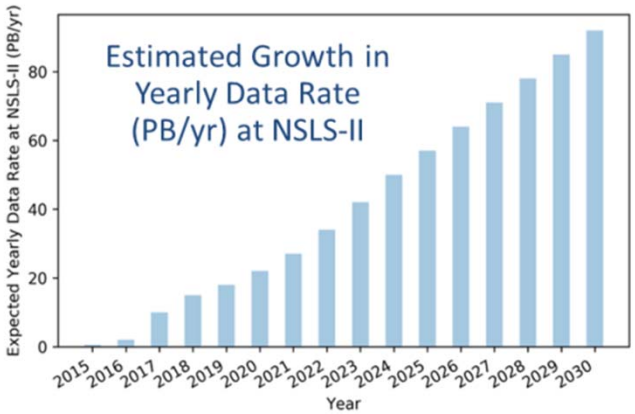
- Continue to improve user experience – streamlined check-in and computer login, easy and secure access to their experimental data during/post experiment
- Continue to expand outreach and education programs – plan to start a new topical summer school for graduate students and early-career researchers, extend graduate lecture to other institutions (*e.g.* InCREASE schools)

Data Acquisition, Management, and Analysis

– Next Five Years

- ***Flexible Modular DAQ Architecture:*** further mature and expand BlueSky open-source DAQ capabilities in collaborations with other BES facilities (SNS, APS, LCLS, …)
- ***Data Broker Application Interface*** retrieves & manages data and metadata. Add role-based security, improved graphical tools, integration of cloud services, and integration with PASS
- ***Multi-tier Data Management System*** (BL local cashe, NSLS-II central, BNL-CSI storage & computing facility): roll out NSLS-II central storage & processing in FY18, and develop and implement plans for long-term data archiving and processing with BNL-CSI
- ***Library of Analysis Software Tools:*** develop analysis tools aligned with NSLS-II beamline development timeline. Codes released under the 'scikit-beam' umbrella to eliminate overlap



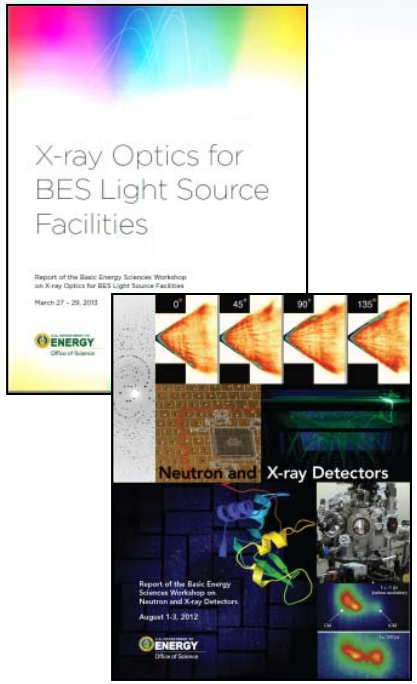


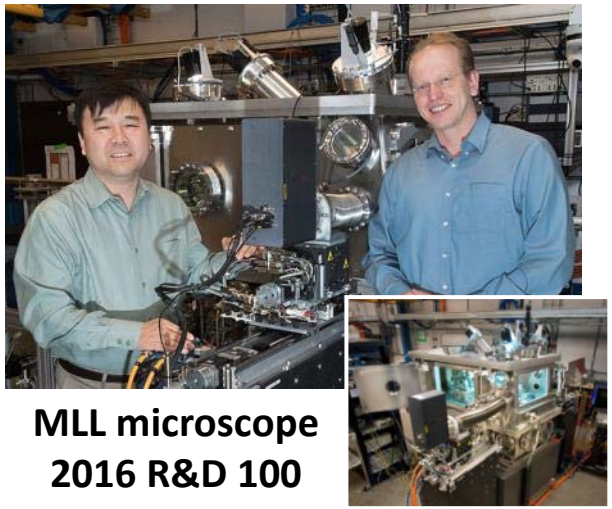
- ***Post-Experiment Data Processing Facility:*** provide front-end computing and centralized data storage/archiving system

Enabling Technology R&D Program

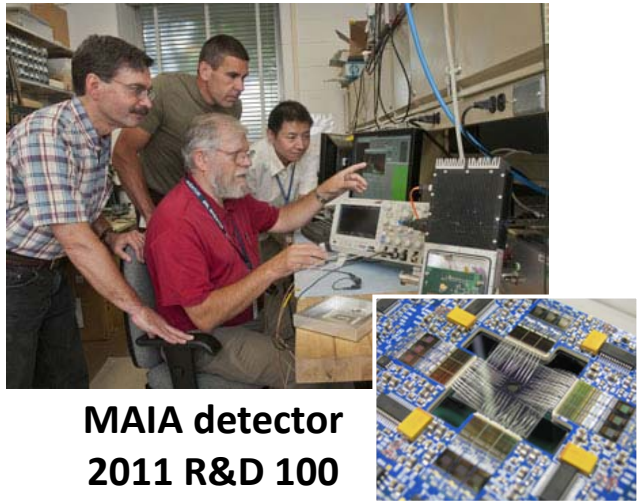
In support of the strategies of DOE-BES Scientific User Facilities, NSLS-II staff pursue R&D

- in targeted technology areas critical to NSLS-II's mission,
- leveraging the strengths and award-winning talents among our staff, and
- in close collaboration and coordination with other Labs





MLL microscope
2016 R&D 100

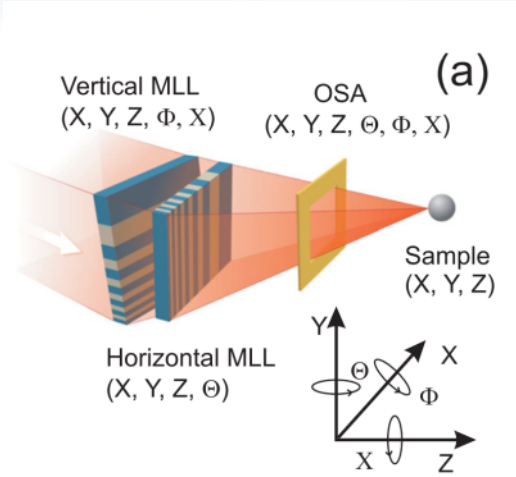


MAIA detector
2011 R&D 100

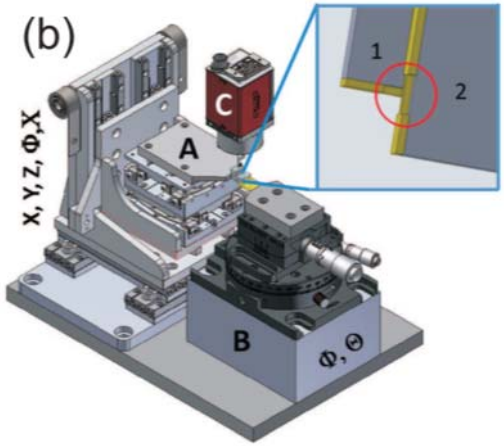
Near-Term Plans & Goals in Optics & Detectors

– Next Five Years

- Nanofocusing Optics: Coordinated R&D plans between APS and NSLS-II being developed through a joint working-group to define complementary R&D programs :
  - MLLs (NSLS-II lead): goal: ~5 nm focus using bonded wedged-MLLs
  - ML-mirrors & stacked ZPs (APS lead): goal: ~10 nm
  - Kinoform lenses (NSLS-II lead): goal: large aperture optics with 250 nm focus for 50 keV x-rays



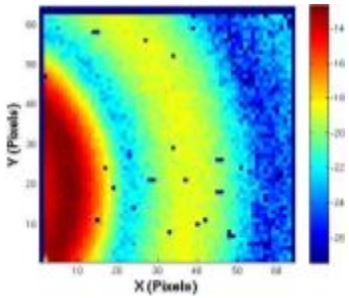
- Hard X-ray Detectors: Continue to develop cutting-edge hard X-ray detectors to support BES-SUF mission, in close coordination with other facilities:
  - MAIA-II: based on LDRD on SDD-based MAIA, we plan to start developing an MAIA-II prototype for spectroscopic imaging in next five years
  - VIPIC: ongoing project; expect to implement this new detector at NSLS-II and at APS XPCS beamlines

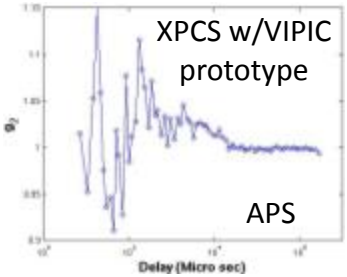


Collaborations on R&D with Other Labs

Closer collaborations among the BES LS facilities in the fields of x-ray technologies will benefit all facilities and will make optimum use of available resources across DOE-BES complex

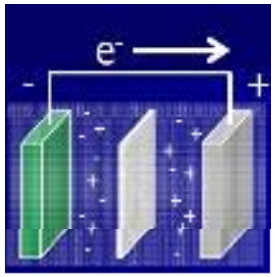
- Optics R&D: APS/NSLS-II working-group report to define complementary R&D program, focusing on two areas: diffractive & refractive optics, and reflective optics
- At-Wavelength Metrology: LCLS/NSLS-II joint project on at-wavelength optical metrology (wavefront sensor) for LCLS-II
- DAMA R&D: APS/NSLS-II/LCLS workgroup to define complementary program in data acquisition, data management, data reduction, data analysis, and data visualization. Next "Hack-a-thon" is at ORNL
- Insertion Devices: coordinating effort with APS in developing new insertion devices *e.g.* SCU and SCW
- Detectors: VIPICS (*Vertically Integrated Photon Imaging Chip)*, and ongoing conversations on detector development for APS-U





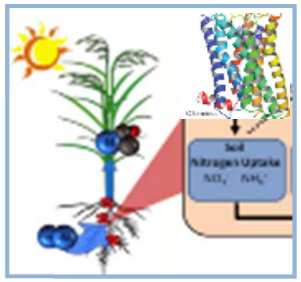
Initiatives and Partnerships

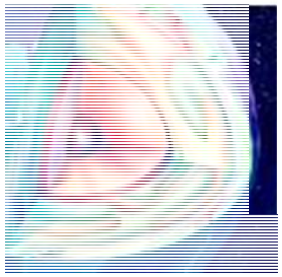
Energy Science



Nanoscience with CFN

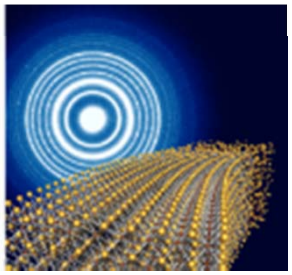
Multiscale Bioscience





Partner Users

Industrial Research

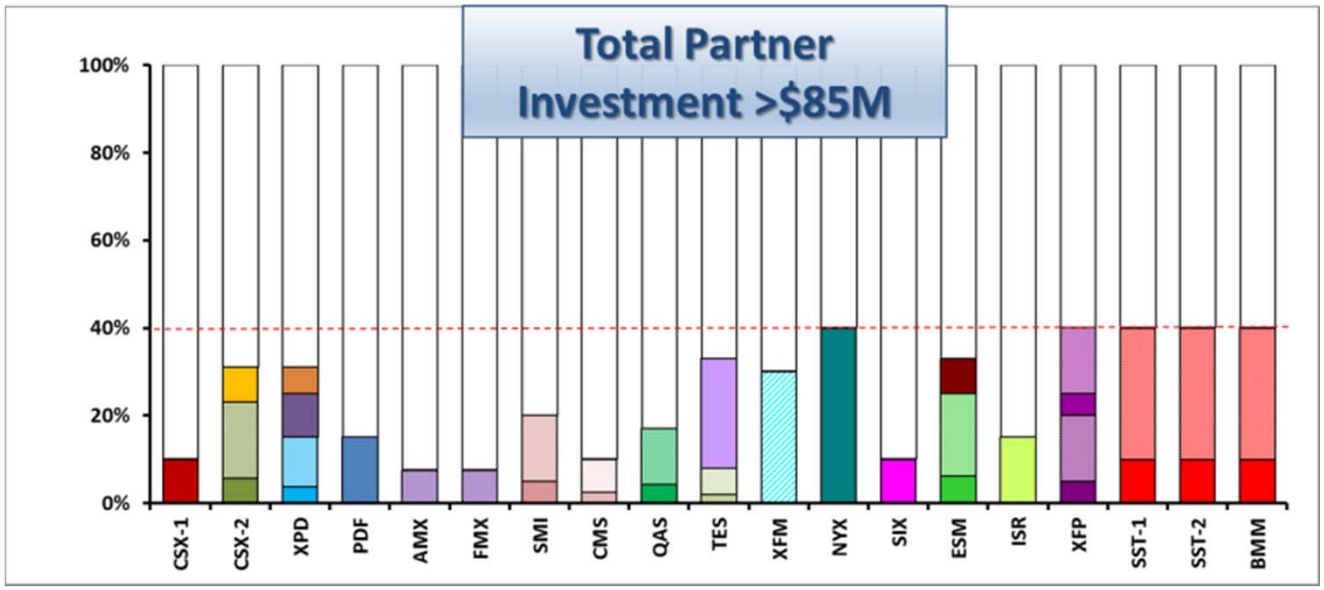


New Initiatives

- We pursue strategic initiatives to leverage interest, intellectual power, and resources in the community to enhance impact of NSLS-II

Initiatives and Partnerships – Partner User (PU) Program

- Objective: to leverage the community interest, expertise, and resources to enable new scientific capabilities and programs at NSLS-II for general users
- PU may contribute cutting-edge instrumentation, new analysis software, and/or specialized staff expertise to bring new capabilities that would not otherwise be present at NSLS-II beamlines
- Early in the process; In FY18 we will evaluate our experience to date as part of our triennial beamline review process

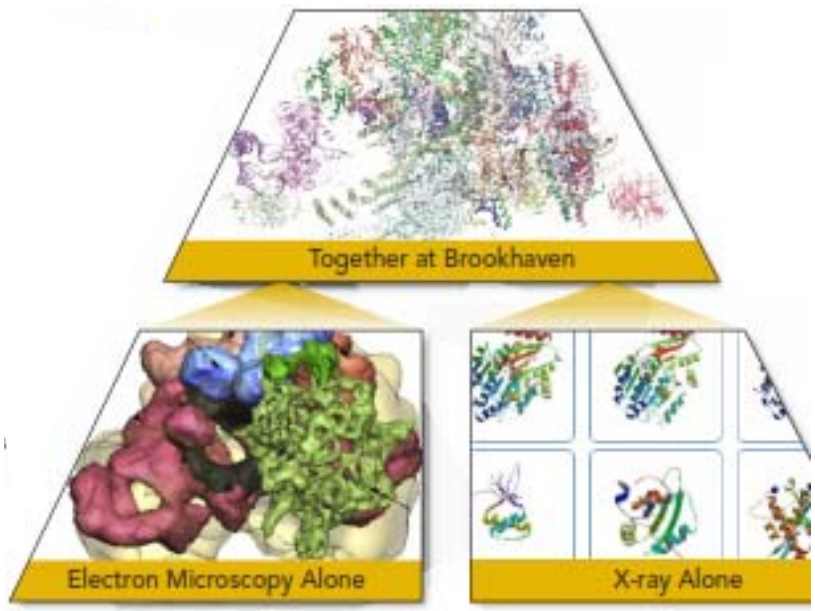


- Current status: 23 PU arrangements at 19 beamlines at NSLS-II:

  Yale, Columbia, Miami U, Boston U, U Vermont, CWRU, NYSBC, NIST, BNL-Chem, BNL-CMPMS, CFN, SCC, COMPRES /Stony Brook, U Chicago

Multiscale Biosciences with Addition of CryoEM

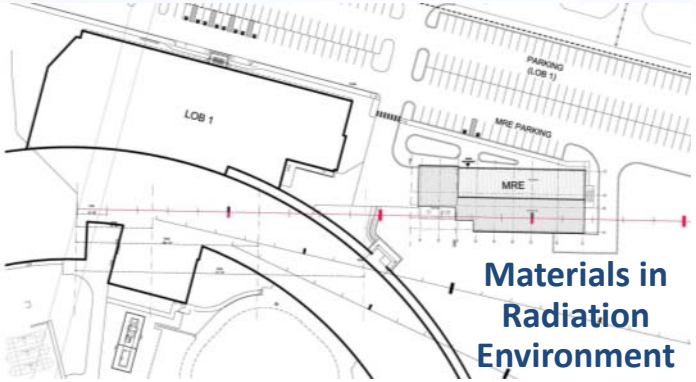
- **Multiscale Synchrotron X-ray Imaging:** Leveraging NSLS-II strength to develop cutting-edge structural and chemical imaging capabilities to enable integrative biosciences at multiscales – from atomic & molecular to cellular & organism scales
- **New Cryo-EM facility:** A beyond state-of-the-art cryo EM user facility, integrating complementary synchrotron x-ray and other techniques to accelerate the solution of large scale biomolecular structures

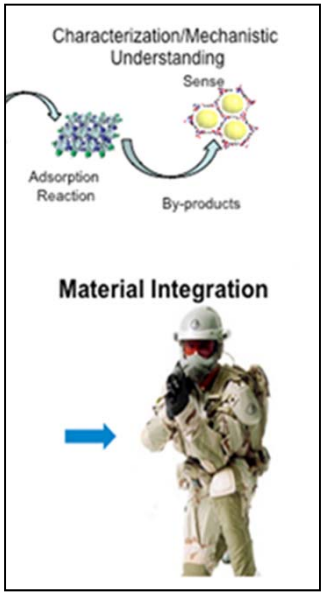


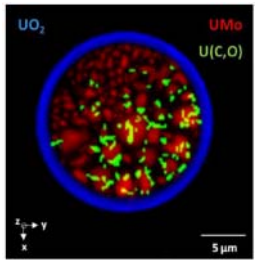
NY State has committed $15 M for the 1st microscope and part of the building

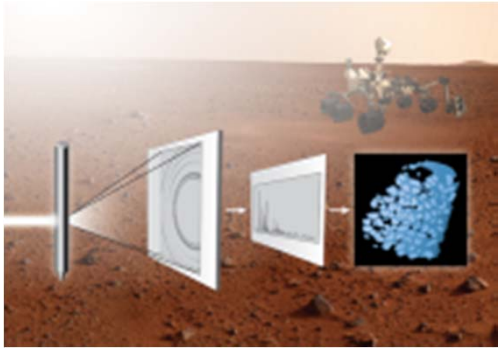
Initiatives to Develop New Communities

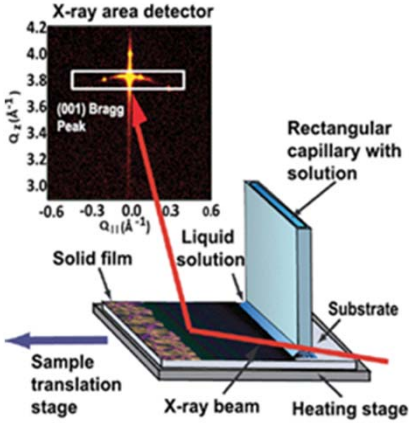
- Outreach to potential new communities that have not been traditional users of synchrotrons
- Current Initiatives on New Communities:
  - Materials in Radiation Environments
  - NASA sample return missions
  - Interagency Advanced Manufacturing Initiative
  - Defense Threat Reduction Agency (DTRA)

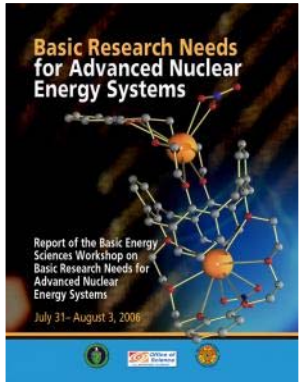












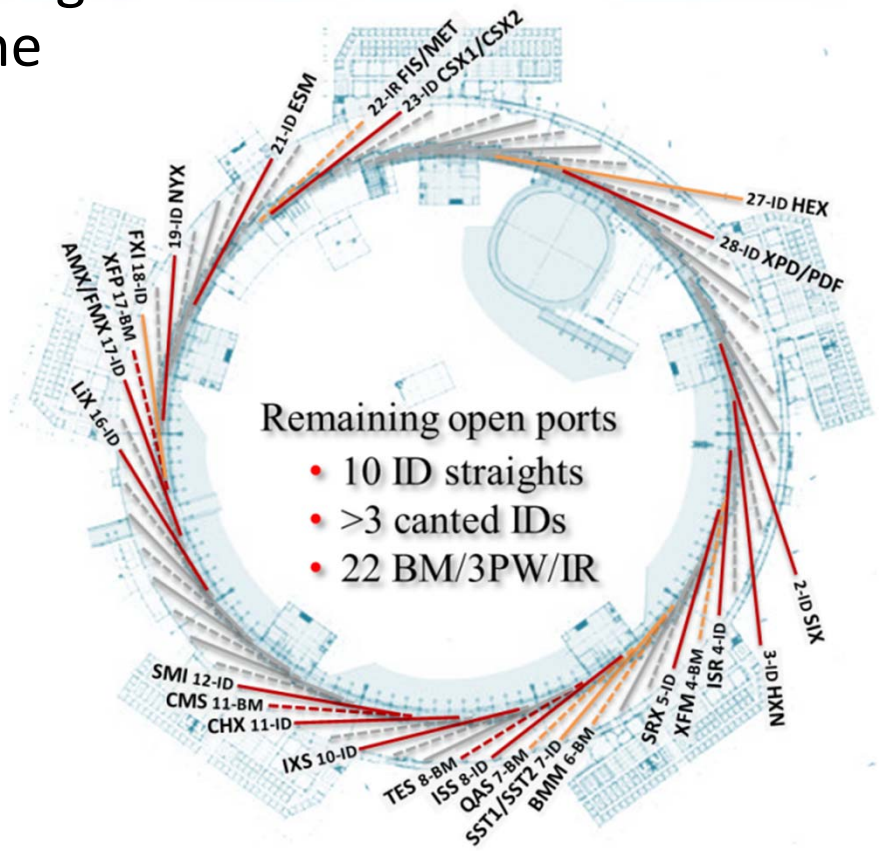
Outline

- Planning process
- Overview of 2017 strategic plan
- Facility improvement plans in next five years
- Beyond next five-years
- Summary

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

Future Beamline Build-out Outlook

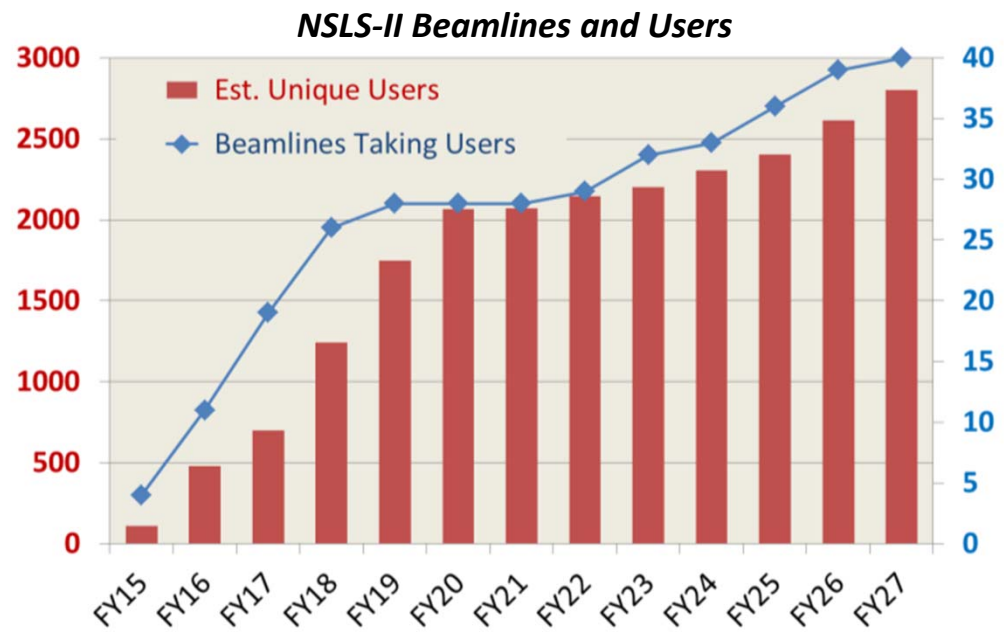
- NSLS-II plans to build out the remaining 10 ID straights as a high priority in the coming 10 years
  → Goal: ~40 BLs in ops by 2027
- Possible beamlines (in addition to the six already identified):
  - Materials in Radiation Environment
  - Beamline in support of DTRA open research
  - Beamline for pharmaceutical industry
  - Parallel branchlines at HEX
  - Coherent scattering dedicated for synthesis
  - Bio-environmental chemical imaging
  - High-throughput micro-tomography
  - NASA sample-return facility
  - ……



- We are having discussions with community and potential sponsors

Vision: NSLS-II in 2027

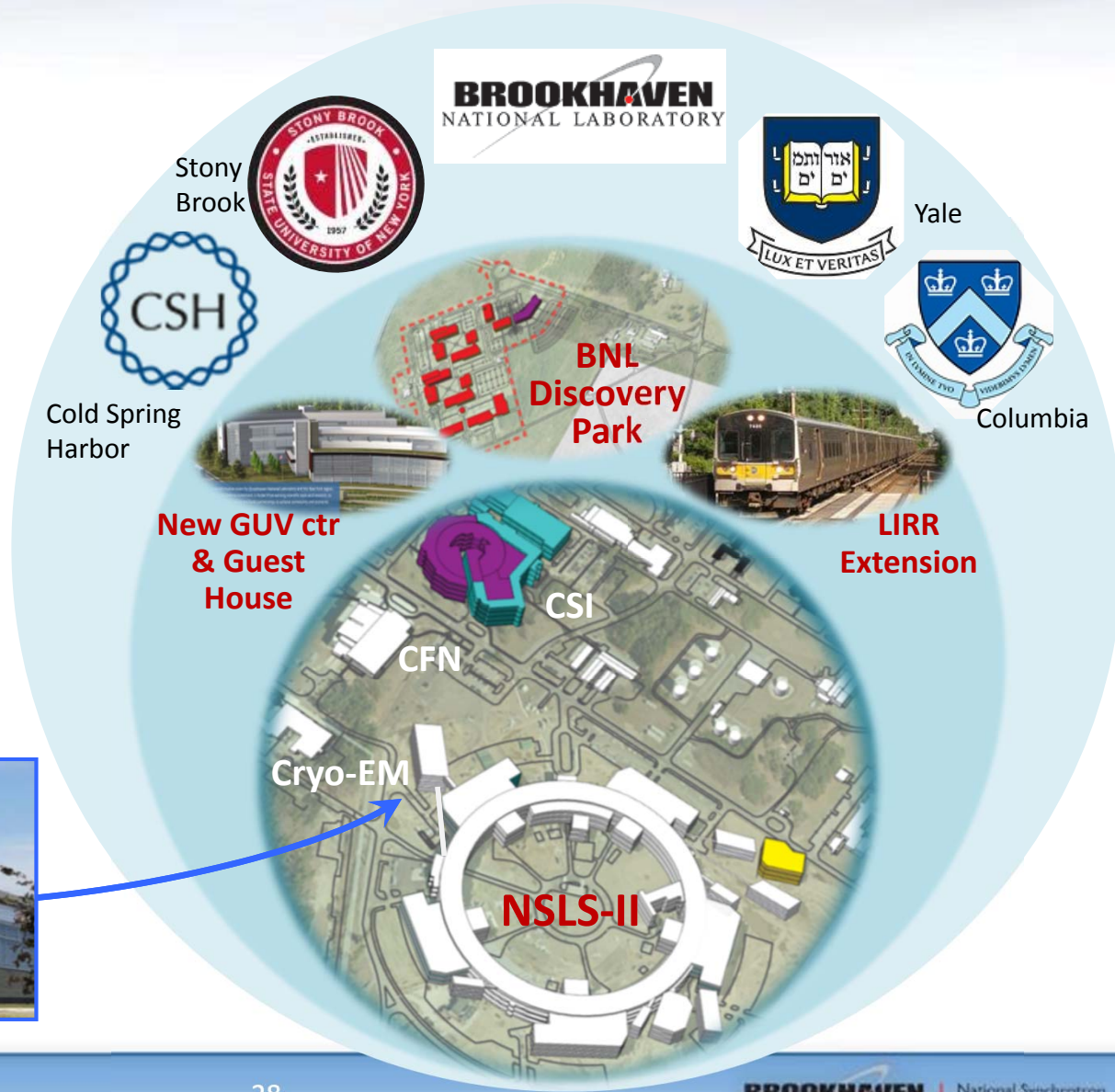
- NSLS-II accelerator system:
  - 2% beam stability with 5000 ops hrs at 500 mA and >95% reliability
  - with optimized superconducting ID's and cryo-IVU's for user programs
  - pursuing an upgrade plan to enhance brightness
- NSLS-II experimental program:
  - operates 40 BLs and cryo-EM facility
  - approaching 3000 users, ~1000 pubs
  - users conducting multimodal, multi-BL, multi-facility, in-situ/operando expts
- NSLS-II data:
  - seamlessly passed to CSI for storage, analysis, and archiving
  - analyzed using suite of software tools during and post-experiment



- NSLS-II R&D:
  - recognized leader in DOE-BES facilities complex in nanofocusing, nanopositioning, hard X-ray detectors
  - next-gen HXN microscope using bonded MLLs with ~5 nm focus in user operations

Vision: NSLS-II in 2027 (cont'd)

- Thriving R&D enterprise with NSLS-II at its center
  - Institutes nucleate around NSLS-II and remote endstations
  - Discovery Park with new GUV center and guest house. Government-private partnership drives innovation and start-ups
  - LIRR increases connectivity
  - Strong partnerships with BNL-SBU-CSHL alliance, with Yale and Columbia, …



Summary

- NSLS-II vision and strategy align well with DOE and other stakeholders' missions and research needs of scientific community
- New *NSLS-II Five-year Strategic Plan* developed
  - with input from SAC and UEC
  - provides guidance for tough budget decisions
  - living document to be updated every year

- Next five years truly exciting for NSLS-II:
  - Ramp accelerator to full performance
  - Ramp-up and mature beamline operations & user programs
  - Complete beamlines in construction and begin to develop new ones
  - Advance R&D critical to DOE/BES scientific user facilities mission
  - Develop data science and computing to maximize productivity
  - Achieve excellence in all aspects of facility operations
- We look forward to working with our stakeholders and community to achieve our 2027 vision