

BNL SBU Workshop on Future of NSLS-II

Structural Biology

Allen M. Orville
Biophysicist, Biology Department

BROOKHAVEN
NATIONAL LABORATORY

a passion for discovery



U.S. DEPARTMENT OF
ENERGY

Office of
Science

“Structural Biologists” at BNL & SBU

BNL NSLS Beamlines & Staff

- **Crystallography (MX)**
X3A, X4A, X4C, X6A, X12B, X12C, X25,
X26C, X29
- **Spectroscopy & Footprinting**
X-ray Absorption Spectroscopy at X3B,
X11A, X11B, X15B
X-ray Footprinting at X28C
- **X-Ray Scattering**
Solution small/wide angle X-ray
scattering at X9, X6B, X27C

BNL Medical Department

- Radiotracer Chemistry,
Instrumentation and Biological
Imaging
- NASA Radiobiology Program
- Cancer Diagnostics & Therapies

BNL Biology Department

- **Bioenergy**
Plant Lipids, Synthesis, & Microbes
- **Structural Genomics**
New York Structural Genomics
- **Biodefense & Disease**
Vaccines, Therapeutics, Diagnostics
- **DNA Damage & Repair**
National Space Radiation Laboratory
Low Dose Radiation Program
- **Molecular Imaging**
STEM; Cryo-EM and Imaging

SBU Departments

- Biochemistry and Cell Biology
- Chemistry
- Pharmacology

Approved Beamlines (to date)

- XFP** X-ray mediated hydroxyl-radical footprinting, probes solvent-accessibility for complexes and their interactions
- XAS** Study freeze-quench intermediates in metalloenzyme reaction cycles and
- LiX** A unique capability is to collect solution scattering data from membrane proteins embedded in membranes.
- ABS** High throughput static solution scattering measurements at the rate of up to one sample per minute
- FMX** MX micro-beam (1 - 50 μm), microcrystals, very large unit cells, will preserve beam coherence
- AMX** MX mini-beam (5 – 300 μm), highly automated to support remote access with multiple simultaneous users
- NYX** MX mini-beam, anomalous scattering from high energy resolution for sharp transitions at resonant edges
- SM3** MX mini-beam, nearly simultaneous spectroscopy and diffraction studies of single crystals

An Example of MX NSLS-II Beamlines

Three canted undulator beamlines

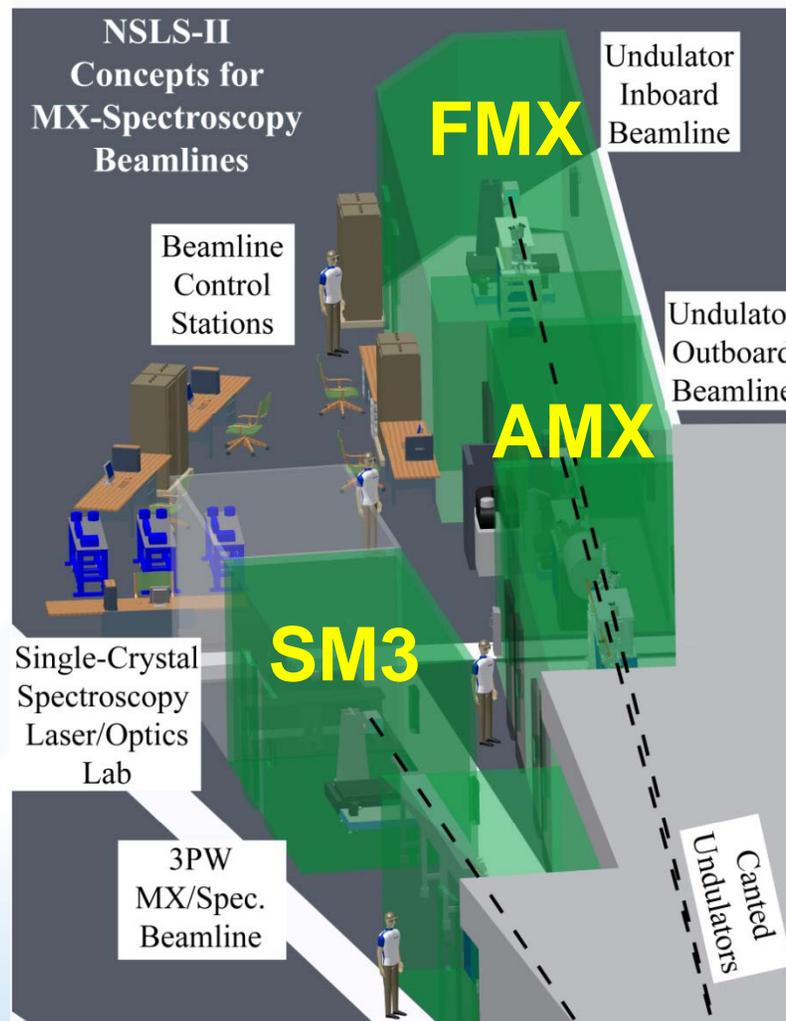
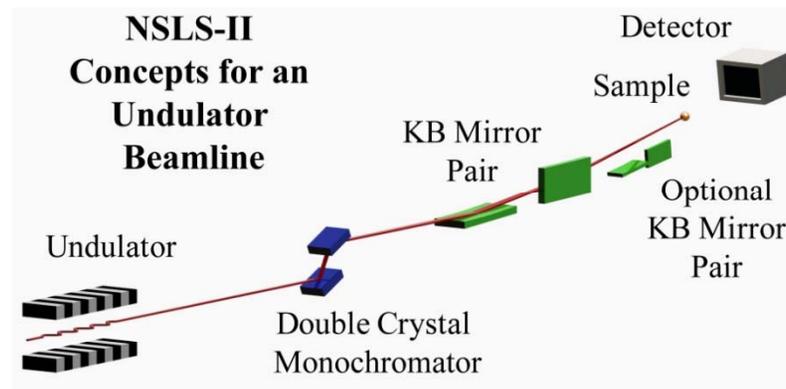
- micro-beam (1 – 50 μm); FMX
- mini-beam (5 – 300 μm); AMX
- mini-beam w/ high res. mono; NYX

A three-pole wiggler beamline

- 25 – 300 μm w/ Spectroscopy; SM3

An off-line laser/optics lab to integrate the spectroscopy + MX capabilities

Missions are aligned well with those of the NIH and the DOE



NSLS-II Structural Biology Beamlines

Approved Beamlines (October 2010)

ABS	A Highly Automated Instrument for Static X-ray Scattering Measurements of Biological Molecules in Solution	Lin Yang, BNL	
LiX	A High-brightness X-ray Scattering Instrument for Biological Applications	Lin Yang, BNL	NIH
AMX	Flexible Access Macromolecular Crystallography at an Undulator Beamline	Dieter Schneider, BNL	NIH
FMX	Frontier Macromolecular Crystallography at an Undulator Beamline	Robert Sweet, BNL	NIH
NYX	NYSBC Microdiffraction Beamline	Wayne Hendrickson, Columbia University	Type 2
SM3	Correlated Single-Crystal Spectroscopy and Macromolecular Crystallography	Allen Orville, BNL	
XAS	X-ray Absorption Spectroscopy for Biological, Environmental and Energy Sciences	Mark Chance, Case Center for Synchrotron Biosciences	
XFP	X-ray Footprinting	Mark Chance, Case Center for Synchrotron Biosciences	

Letters of Intent (2011 Call for Beamline Development Proposals)

HIT	Synchrotron-based discoveries for Chemical Biology	Marc Allaire, BNL
LAX	Low-energy Anomalous X-ray Diffraction Beamline	Wayne Hendrickson, Columbia University
HMX	High Energy MX beamline	Vivian Stojanoff, BNL