X-RAY SCIENCE DIVISION FY2021 PRIORITIES
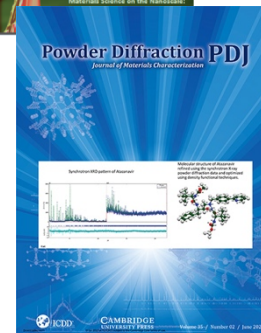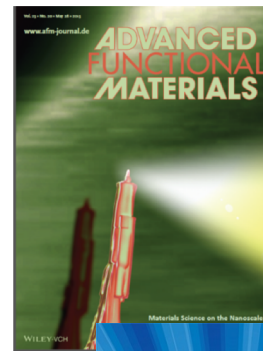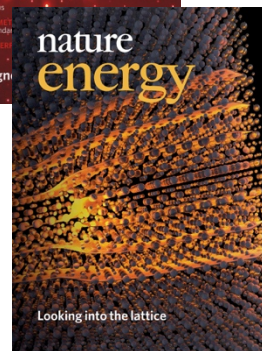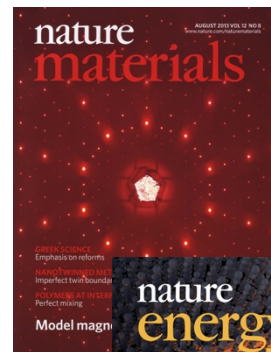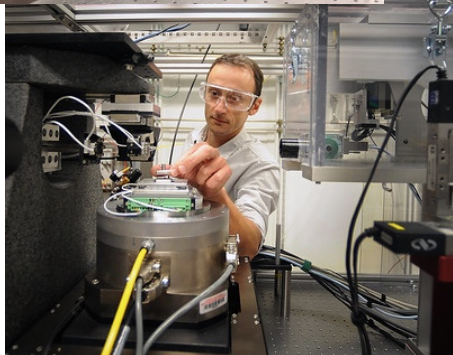
JONATHAN LANG
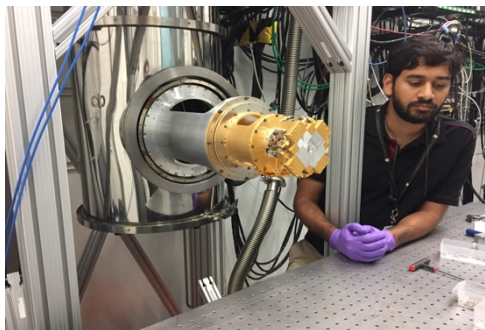X-ray Science Division
Photon Sciences Directorate

APS All-Hands Meeting
August 3, 2020

X-RAY SCIENCE DIVISION - MISSION

Enable and conduct world-class research using x-rays by developing cutting-edge x-ray instrumentation and techniques.
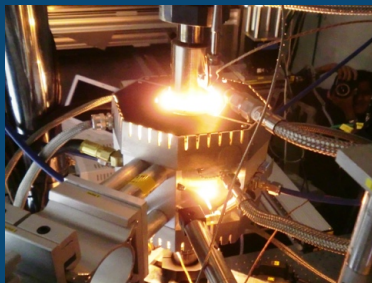

Operate 44 (35 + 9) of 68 beamlines; partner in 1 additional beamline

APS CY19: **2008** (1079 + 290) **publications** ~17% high impact; > 5700 users

X-RAY SCIENCE DIVISION STRATEGY

High Energy
Penetrating bulk materials and operating systems
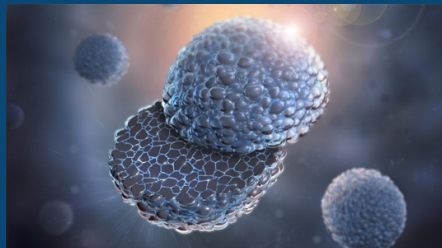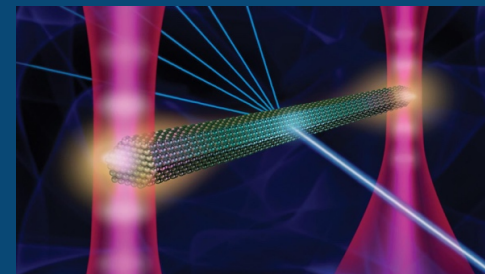
Brightness/Coherence
Highest possible spatial resolution/dynamics
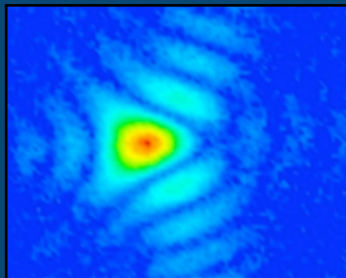
Time-Resolved Studies
Measurements from ~100ps to seconds
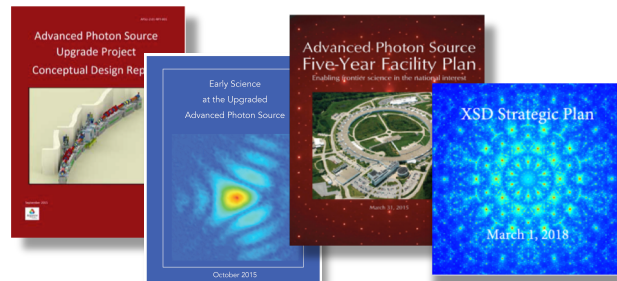
Argonne National Lab
Leverage ANL core research programs & advanced computing facilities to enhance x-ray capabilities & scientific productivity

Make the APS will be the premier light-source for brilliance driven high-energy x-ray measurements post-upgrade

X-RAY SCIENCE DIVISION STRATEGY

Leverage unique characteristics of APS & ANL.

- Enhance and expand core capabilities related to APS-U
  - High-Energy, Nanofocusing, Coherence, Imaging, …
- Develop optics, detectors, instruments, and data strategies relevant to APS-U
- Foster effective lab & external partnerships to improve APS capabilities & strengthen ANL research.
- APS-U/APS beamlines
  - APSU "feature" beamlines & beamline "enhancements"
  - Strategic investments to full APS beamline suite.
- Operate suite of world-class x-ray capabilities for the US scientific community.

Simulated Measurement | Recovered
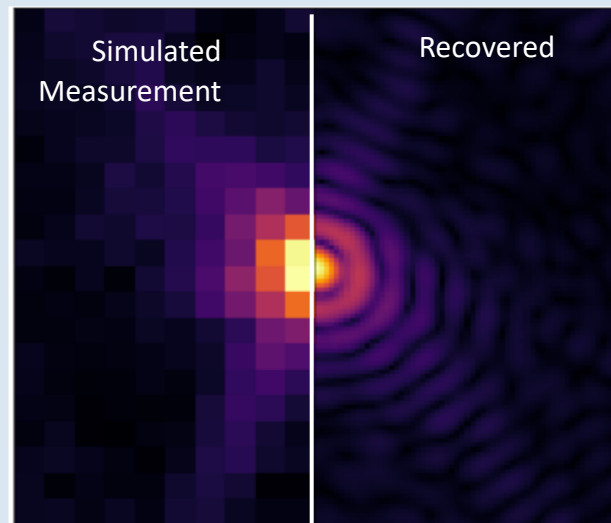
Coherent imaging at 54 keV. Left: coarse pattern due to compression of reciprocal space, Right: recovered pattern using oversampling method
S. Maddali et al., Sci Reports 8, 4959 (2018)

RECENT PROGRESS

- High-Throughput HEDM instrument installed at 6-ID-D (NSF; Carnegie Mellon; XSD – MPE & MM)

- LYNX ptychographic laminography instrument successfully tested at 33-ID (iARPA / XSD-MIC)

- Successful demonstration of 1D Zoom Optics for controllable beam size at the sample position

- Deployed and tested high-energy transition edge sensor detector at 1-BM

- Number of projects initiated to apply AI/ML & HPC for spectroscopy, synthesis, CDI, …
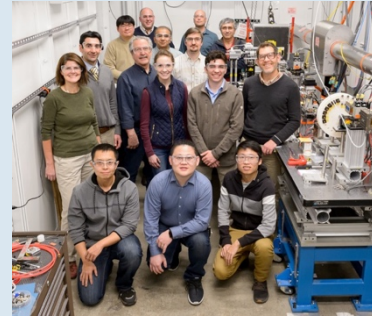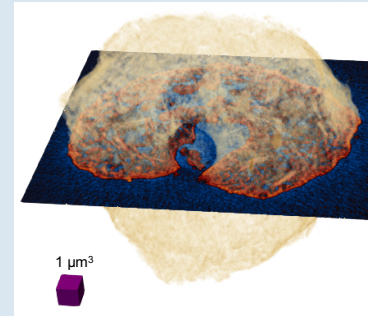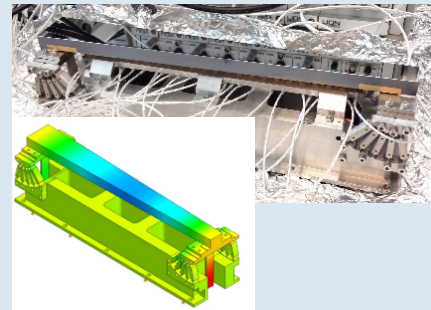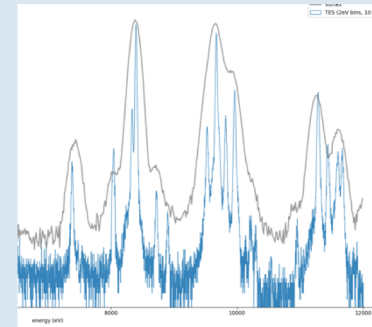

HT-HEDM team at 6-ID-D, Dec. 2019


1 µm³

Image of zeolite catalytic particle using LYNX at 33-ID

Flexure based mirror bender with capacitive sensor readback

Spectroscopy scans with TES & Ge SSD detector

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XSD FY21 BEAMLINE TECHNOLOGIES

- Upgrade APS metrology lab to be APS-U ready.
  - Long Trace Profiler
  - Interferometer and stitching software
- Mixed Mode PAD Detector (APS/Cornell)
  - High dynamic range (10^8), high-speed (>1kHz), high-energy detector (CdTe sensors).
- Develop HPC tools for fast (real-time) analysis
  - Continue to strengthen ties with ASCR programs to develop analysis pipelines and on-demand queues
- Advanced experiment control
  - Enable additional remote access capabilities
  - Continue expanding Bluesky (NSLS-II) deployment on XSD beamlines
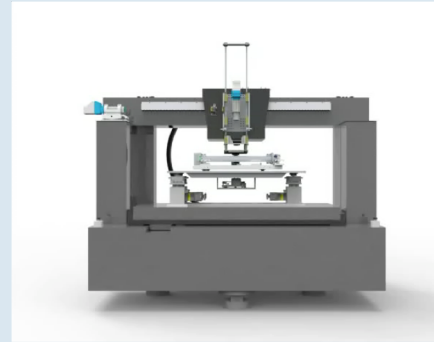
Long Trace Profiler upgrade

MM-PAD v2 prototype
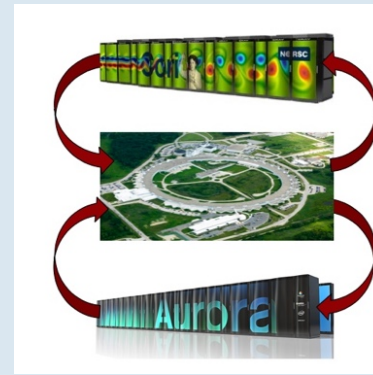
HPC data analysis

Remote operation of 34-ID-C

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XSD FY21 BEAMLINE PROJECTS
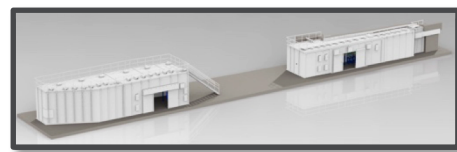
- Work to enable additional automation and remote operations on XSD beamlines

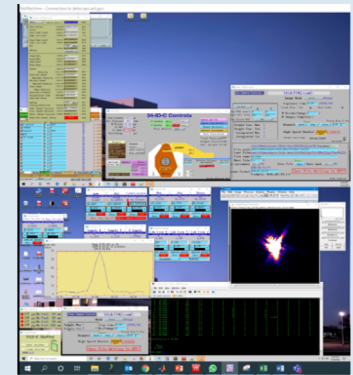- Work with APS-U on completion of the buildout of IDEA (28-ID) and ASL (25-ID) beamlines, and start of POLAR (4-ID)

- Complete LYNX instrument commissioning for ptychographic imaging of integrated circuits at 33-ID & 7-ID, install at 28-ID once ready.

- Complete canting work at 2-ID beamline to rationalize spectromicroscopy capabilities and prepare for APS-U

- Continue development of AI and ML approaches for data analysis and rapid experimental feedback at the beamlines (CDI, XES, Materials synthesis, …)

A.I. CDI
Atomistically Informed Coherent Diffraction Imaging

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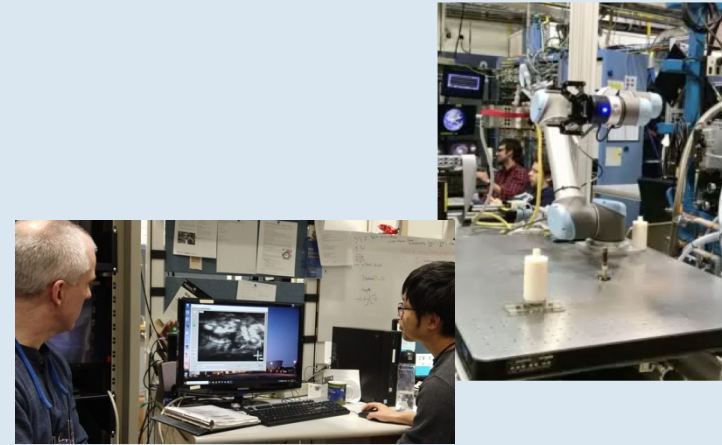
X-RAY SCIENCE DIVISION FY21 GOALS

- Facilitate active and productive user programs by pivoting towards increased automation and remote operations on XSD beamlines

- Develop innovative instrumentation that further advances beamline capabilities particularly for high-energy, coherence, nano-focusing, ….

- Complete current beamline development projects
  - Canting 2-ID to rationalize spectro-microscopy
  - APS-U IDEA & ASL beamlines (25-ID & 28-ID)
  - APS-U start construction of POLAR beamline at 4-ID

- Upgrade of metrology capabilities to support APS-U

- Continue to attract, develop, and retain a diverse set of talented scientific and technical staff.

- Work with staff on addressing challenges brought on by pandemic & accomplishing work in a safe manner

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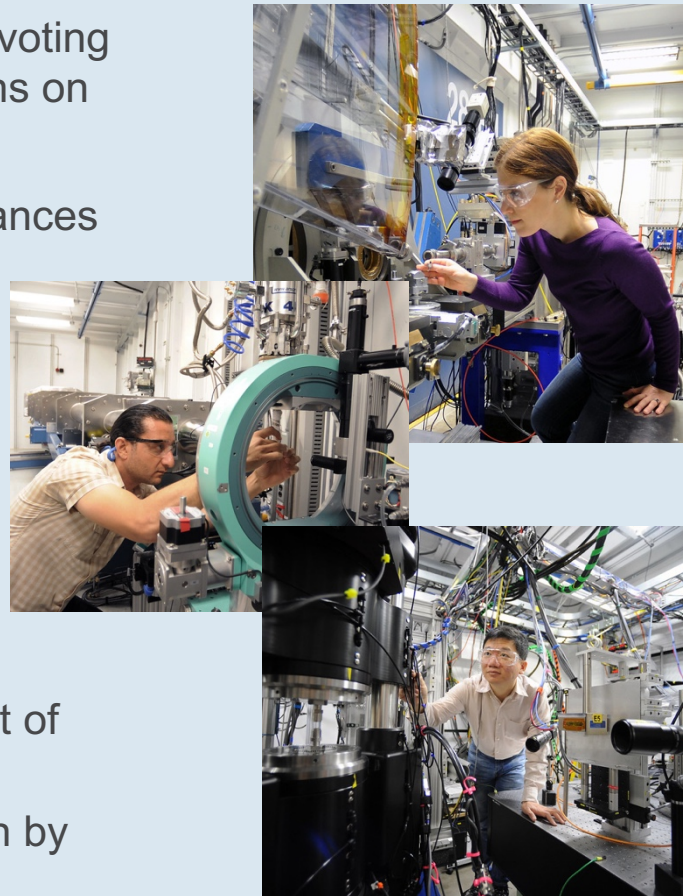
ARGONNE IMPACT AWARDS

- *For conducting and enabling forefront research funded by the Center for Structural Genomics of Infectious Diseases (CSGID) on the expression, crystallization, and structure determination of 29 COVID & COVID related proteins*

  Paula Boudin, Changsoo Chang, Michael Endres, Robert Jedrzejczak, Andrzej Joachiamiak, Youngchang Kim, Alex Levens, Krystof Lazarski, Natalia Maltseva, Karolina Michalska, Jerzy Osipiuk, Michelle Radford, Darren Sherrell, Lucy Stols, Kemin Tan, Chris Tesar, Mateusz Willamowski,(XSD-SBC) Maria Lesnicki, Ana Zavala, Ron Moore (IS)
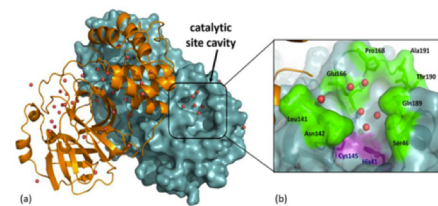
RT structure of 3CL M^{pro} protease Daniel Kneller *et al*., *Nat. Comm.* **11**, 3202 (2020)

- *For support of COVID and other vital medical research at GMCA, rapid transition to new operating mode, and compiling essential data for DOE reporting on APS COVID work.*

  Kristen Ahrens, Michael Becker, Steve Corcoran, Dale Ferguson, Mark Hilgart, David Kissick, Oleg Makarov, Craig Ogata, Sergey Stepanov, Nagarajan Venugopalan, Shenglan Xu, Qingping Xu (XSD-GMCA).
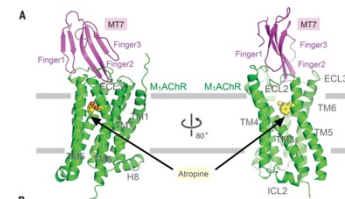
Structure of muscarinic receptor toxin Shoji Maeda *et al*., *Science* **369**, 161 (2020)

Thank You

ARGONNE IMPACT AWARDS

- *For rapid development of electro-spun nanofiber materials for use as filters in N95 masks by National Virtual Biotechnology Lab (NVBL).*

  Vincent De Andrade, Viktor Niktin, Francesco De Carlo, (XSD-IMG), Yuepeng Zhang, Devon Powers, Krysztof Pupek, Benjamin Gould, … (EGS-AMD)

- *For collaborative work that laid the foundation for and resulted in ANL receiving the Scinet Technology Challenge Prize at SC19*

  Tekin Bicer, Zhenchung Liu (CELS-DSL) , Vincent De Andrade, Francesco De Carlo, Junjing Deng, Doga Gursoy, Jeff Klug, Pavel Shevchenko, Stefan Vogt (XSD), Ian Foster, Raj Ketimuthu, Mike Papka, Stefan Wild (CELS), Jim Chen, Joe Membretti (NU)

- *For effort involved in upgrading and reconfiguring the HPCAT computer network.*

  Arun Bommanavar, Richard Ferry, Eric Rod (XSD-HP), Mark Engbretson (XSD-BC), Zacharey Basile, Clarence Clark, Daniel Devito, David Leibfritz, Troy Lutes, Vincent Nobels, Brian Pruitt, David Wallis, Mary Westbrook, Ed Wrobel (AES-IT).
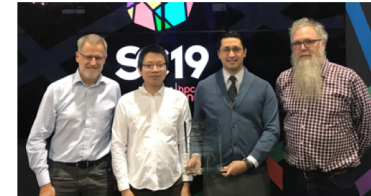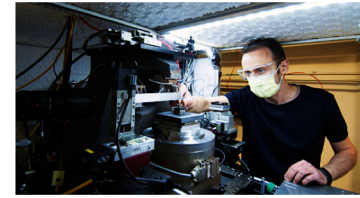
Thank You Argonne NATIONAL LABORATORY

X-RAY SCIENCE DIVISION