WELCOME & OVERVIEW

ADVANCED PHOTON SOURCE (APS)

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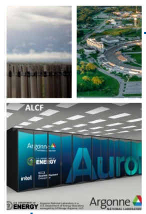
Associate Laboratory Director for Photon Sciences
Advanced Photon Source Director

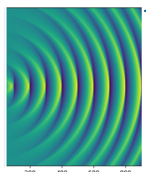
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

OUTLINE

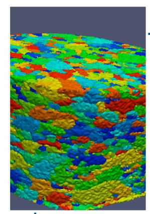


1. Introduction to Argonne and APS

2. Basic principles of synchrotron radiation



3. Characteristics of synchrotron light



4. Types of experiments/science

5. The APS-Upgrade

ARGONNE NATIONAL LABORATORY

Contractor
- UChicago Argonne LLC

Physical assets
- 1,517 acres
- 156 buildings

Human capital
- 3,500 FTE employees
- 500+ students
- 8,035 facility users

Location
- Lemont, Illinois, near Chicago

Type
- Multiprogram laboratory

We integrate our domain strengths to achieve impactful team science and engineering

Advanced Energy Technologies

- Applied materials
- Energy systems and infrastructure analysis
- Transportation and power systems

Computing, Environment & Life Sciences

- Applied mathematics & computer science
- Computational science
- Data science & learning
- Biosciences
- Environmental science

Physical Sciences & Engineering

- Chemical sciences & engineering
- Materials science
- Nanoscience & nanotechnology
- Nuclear & particle physics

Photon Sciences

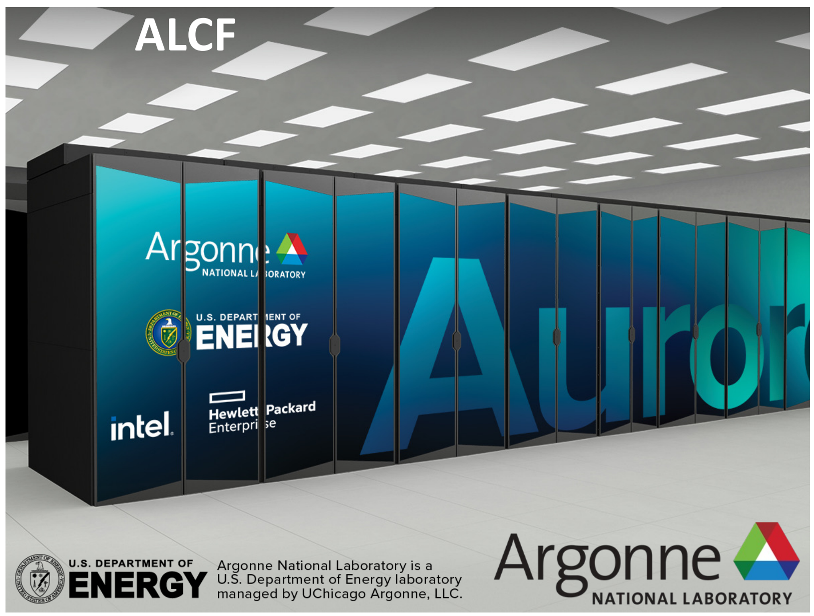
- X-ray science
- APS
- Accelerator systems & engineering

Nuclear Technologies and National Security

- Chemical & fuel cycle technologies
- Decision & infrastructure sciences
- Nuclear science & engineering
- Strategic security sciences

Science and Technology Partnerships and Outreach


ARM

APS

ALCF
intel
U.S. DEPARTMENT OF
ENERGY
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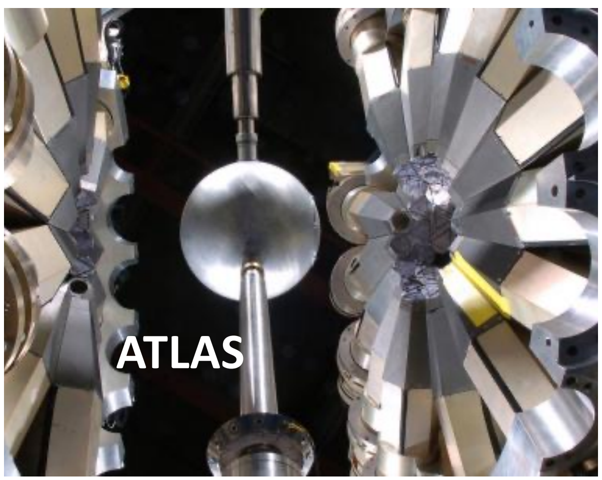
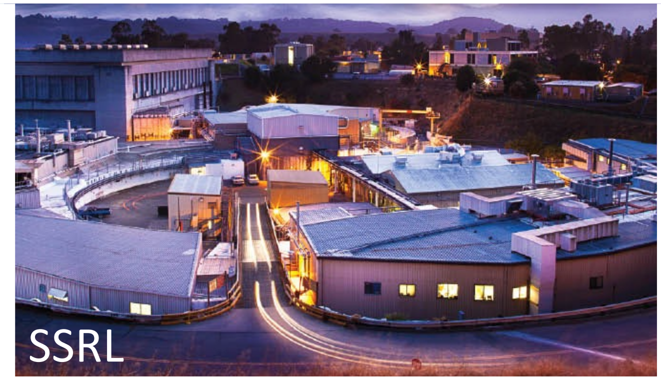
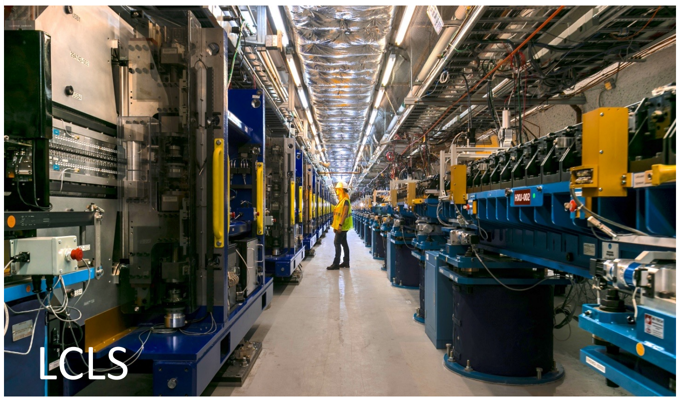
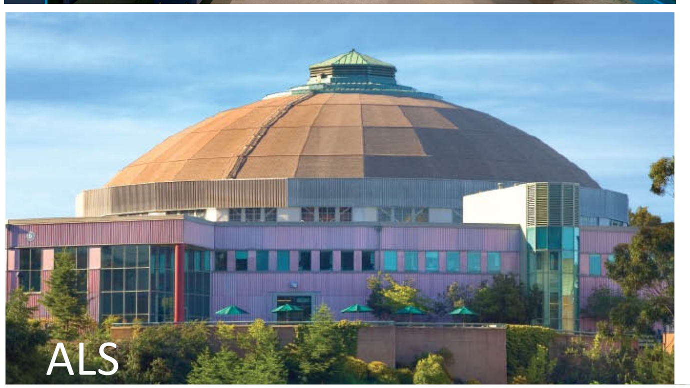
Argonne
NATIONAL LABORATORY

ATLAS

CNM







Basic Energy Science – DOE light sources

U.S. DEPARTMENT OF ENERGY
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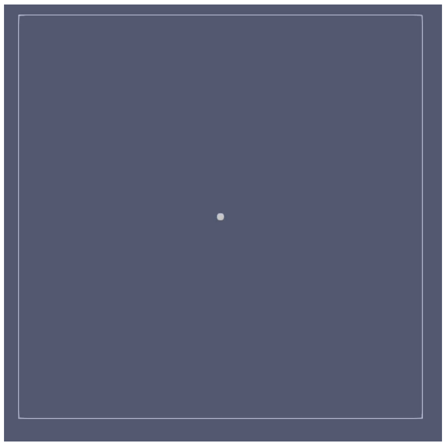
Argonne NATIONAL LABORATORY

RADIATION FROM ACCELERATED CHARGES

From β=0 to β~1 $(\beta = \frac{v}{c})$



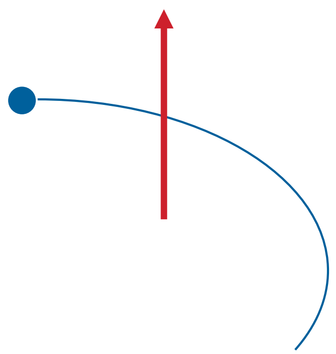
E-field from accelerated charge

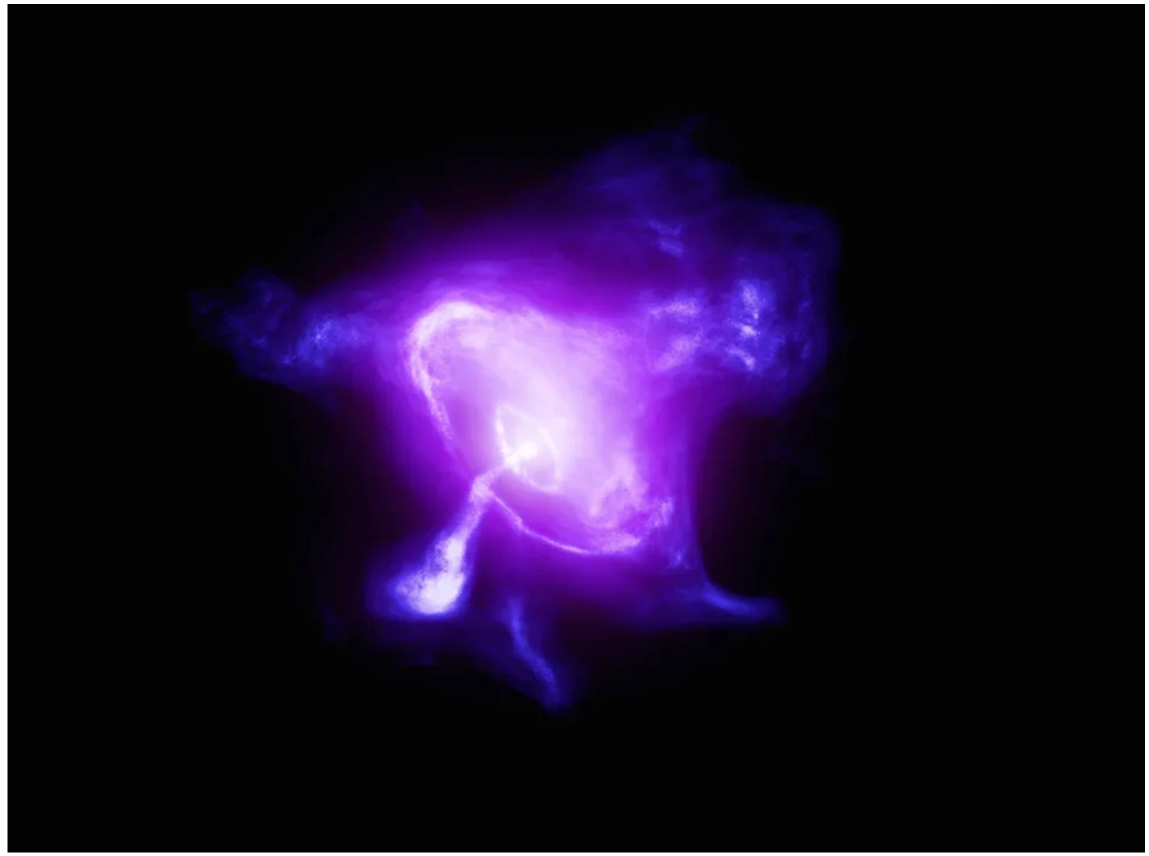
$$\vec{E} = \frac{q}{4\pi\epsilon_0 c(1-\vec{\beta}.\vec{n})^3}\frac{\vec{n}\times(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}}{R}$$

Jackson "Classical Electromagnetism"

SYNCHROTRON RADIATION IN ASTRONOMY

$$\vec{F} = q\left(\vec{E} + \vec{v}\times\vec{B}\right)$$

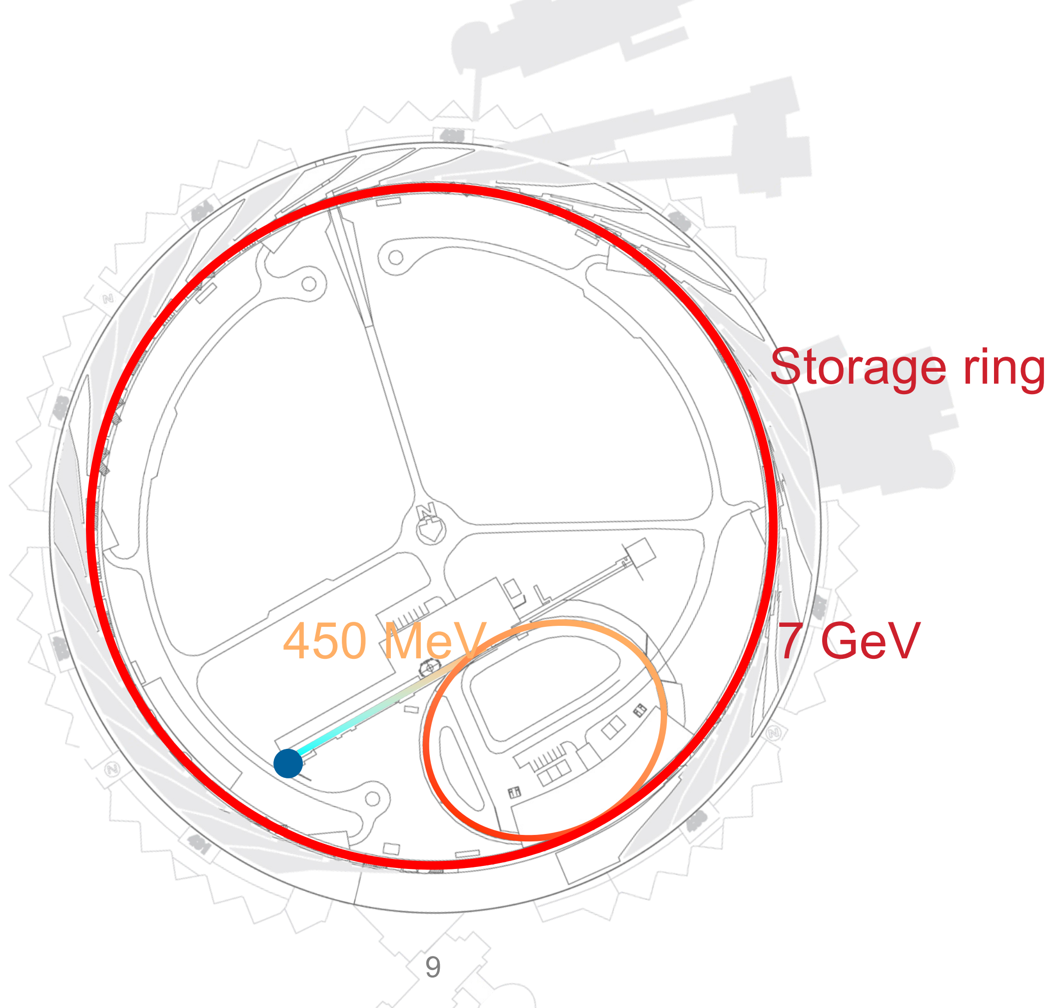




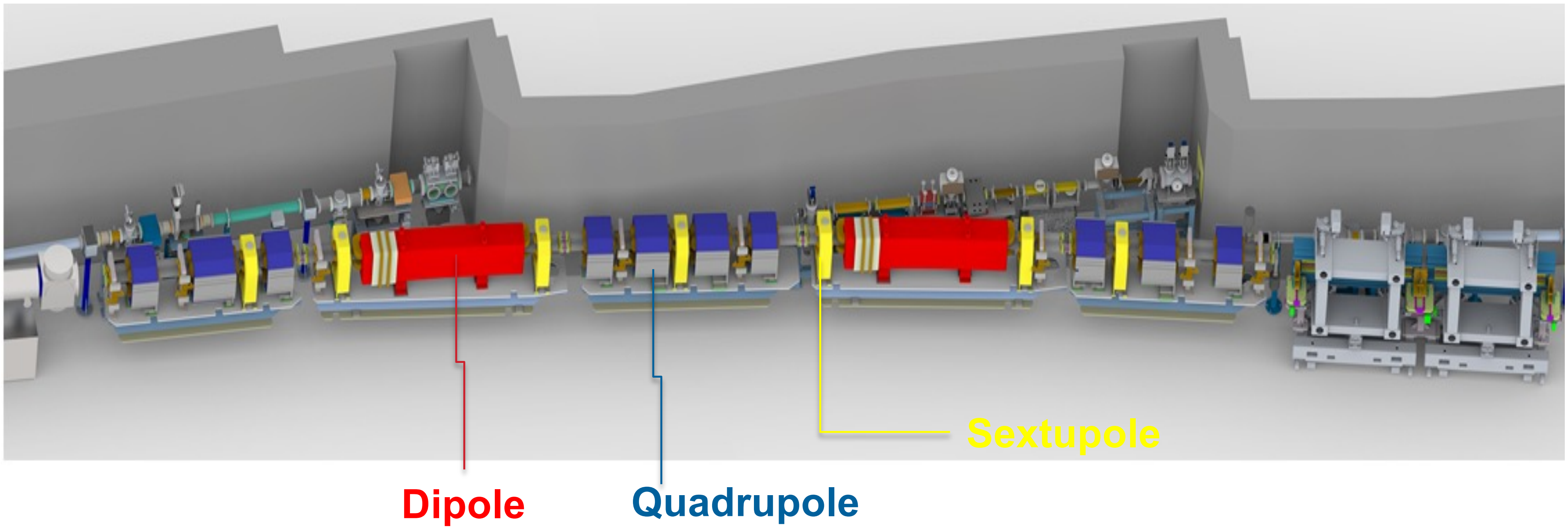
NASA's Imaging X-ray Polarimetry Explorer (IXPE) in magenta and NASA's Chandra X-ray Observatory in dark purple

X-RAY SYNCHROTRON - BASICS

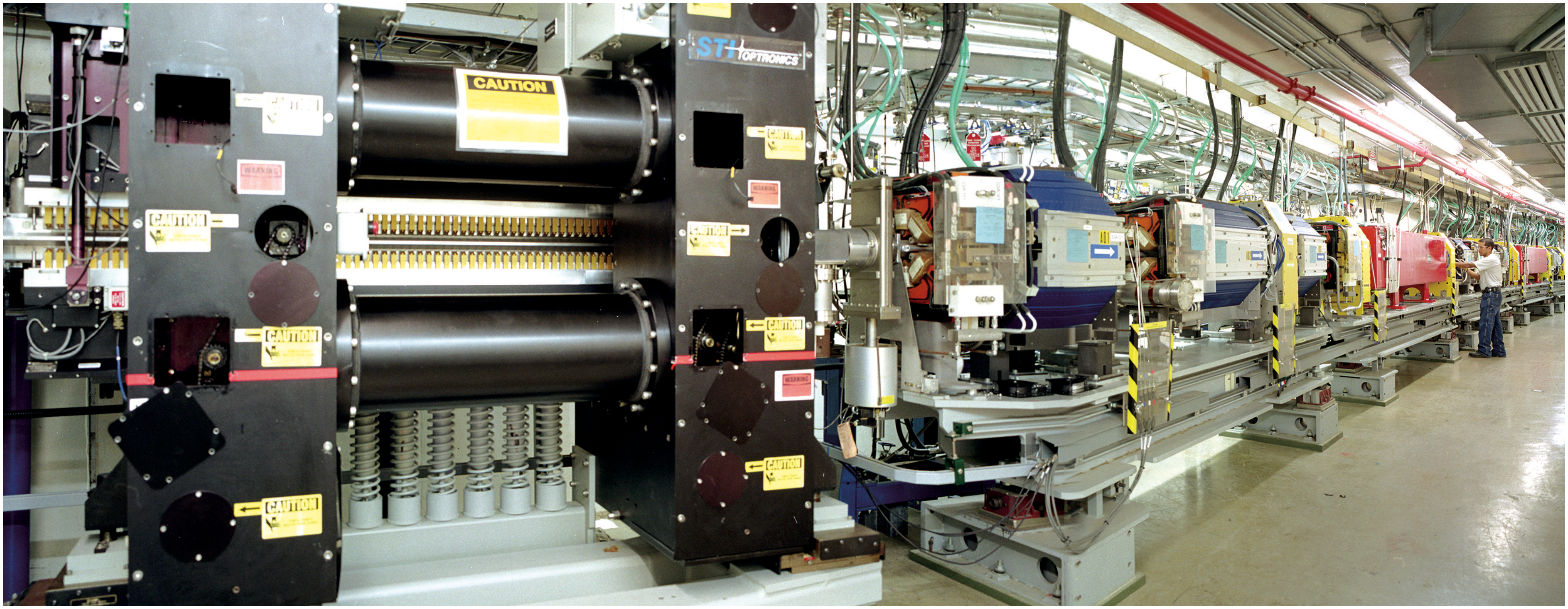
$$m_e = 0.511\ MeV$$



MAGNETIC LATTICE



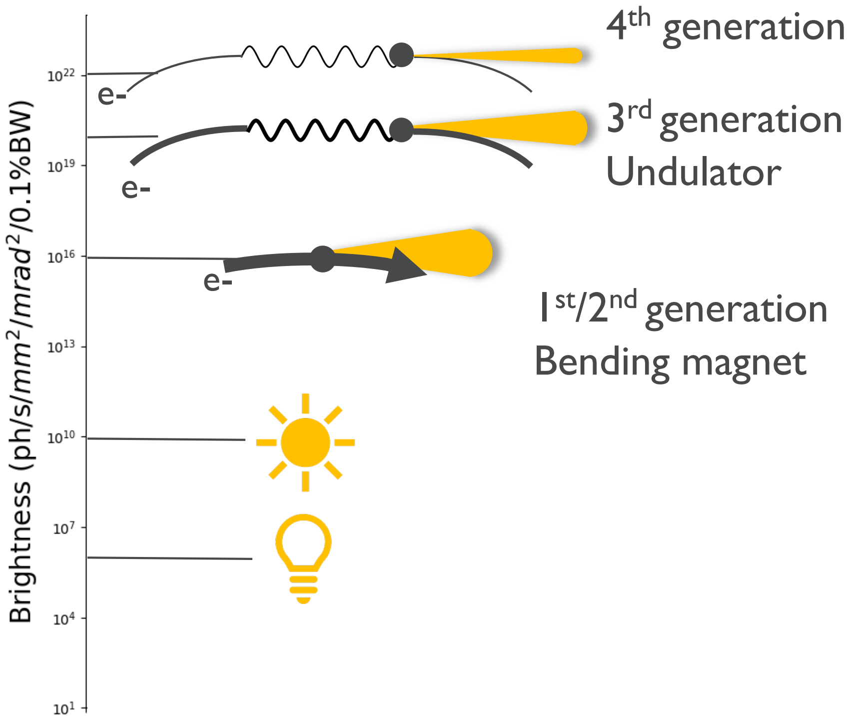
Typically : Several billion electrons per bunch



APS storage ring

SOURCES

Generations of synchrotrons



Flux

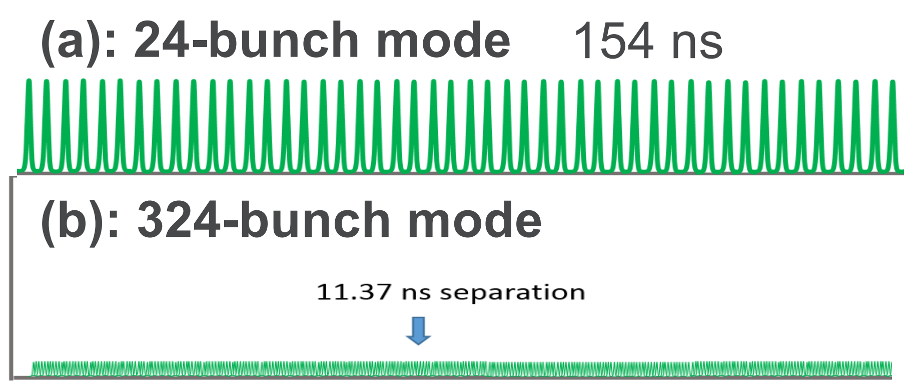
$$\Phi = \frac{n_{ph}}{\Delta t \cdot \frac{\Delta\omega}{\omega}}$$

Spectral brightness

$$\mathcal{B} = \frac{\Phi}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_y \Sigma_{y'}}$$

PROPERTIES OF SYNCHROTRON RADIATION

- **High brightness.**
- **Wide energy spectrum:** from 10s of eV to >100 keV.
- **Tunable energy**
  – Elemental sensitivity by tuning to specific absorption edges
- **Highly polarized radiation**
  – Which can be manipulated
- **Coherence**
  – High degree of spatial and longitudinal
  – coherence
- **Short pulses, typically ~100 ps**
  – Different filling patterns

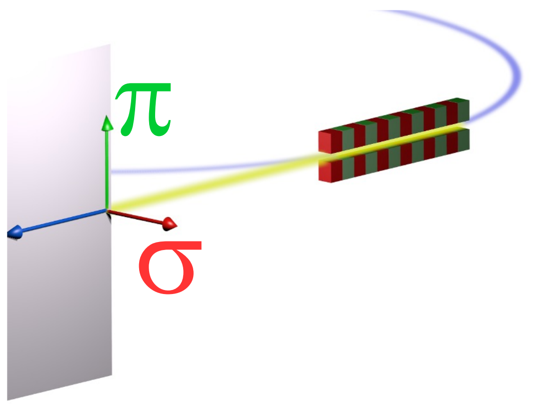


POLARIZATION

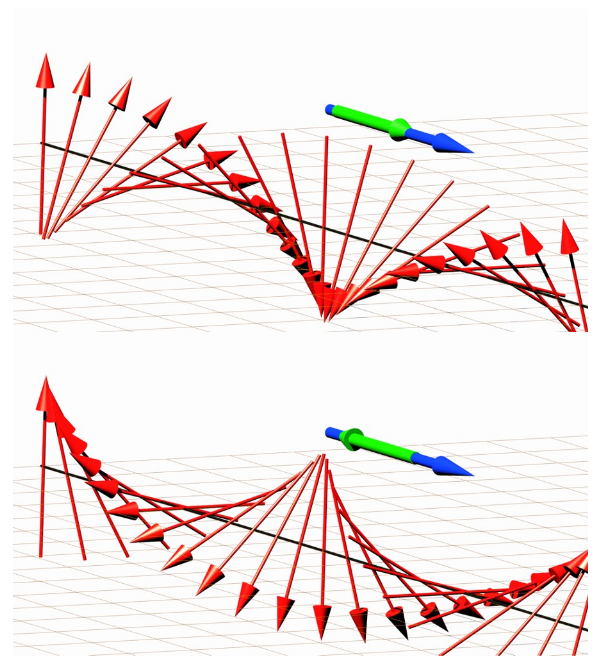
- Naturally polarized in the horizontal plane with a planar undulator

E-field from accelerated charge

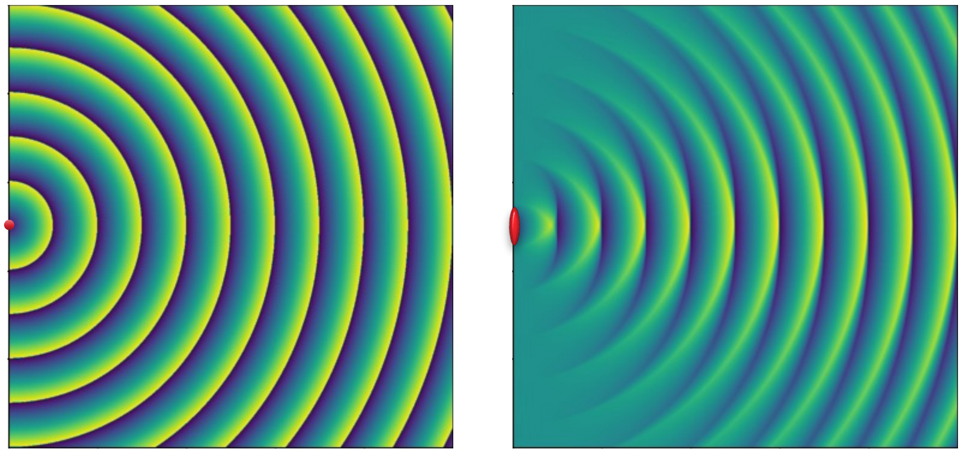
$$\vec{E} = \frac{q}{4\pi\epsilon_0 c(1-\vec{\beta}.\vec{n})^3}\frac{\vec{n}\times(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}}{R}$$



- The polarization can be manipulated by either Undulators directly or phase plates



SPATIAL COHERENCE



Spatial coherence from ducks
https://physicstoday.scitation.org/doi/pdf/10.1063/1.3366225
https://www.youtube.com/watch?v=4o48J4streE

X-RAYS COUPLE TO CHARGE, AND TO SPIN

Hamiltonian electron in EMF

$$\mathcal{H} = \sum_j \frac{(\boldsymbol{p_j} + e\boldsymbol{A}(\boldsymbol{r_j}))^2}{2m}$$ Kinetic

$$+ \frac{e\hbar}{2m}\boldsymbol{\sigma_j} \cdot \vec{\boldsymbol{\nabla}} \times \boldsymbol{A}(\boldsymbol{r_j})$$ Zeeman

$$+ \frac{e\hbar}{2(2mc)^2}\boldsymbol{\sigma_j} \cdot [(\boldsymbol{p_j} + \boldsymbol{eA}(\boldsymbol{r_j})) \times \partial_t \mathbf{A_j} - \partial_t \mathbf{A_j} \times (\boldsymbol{p_j} + \boldsymbol{eA}(\boldsymbol{r_j}))]$$ SO coupling

$$+ \sum_n V_{jn}$$ Coulomb

$$+ \sum_{\boldsymbol{k},\epsilon} \hbar\omega_k \left(a^\dagger_{\boldsymbol{k},\epsilon} a_{\boldsymbol{k},\epsilon} + \frac{1}{2} \right)$$ EMF self-energy

ADVANCED PHOTON SOURCE

- Highest Energy: 7 GeV
- High Brilliance
  - ✓ Small beams (≲μm) & Coherence
- Unique timing structure
- Polarized in the horizontal plane

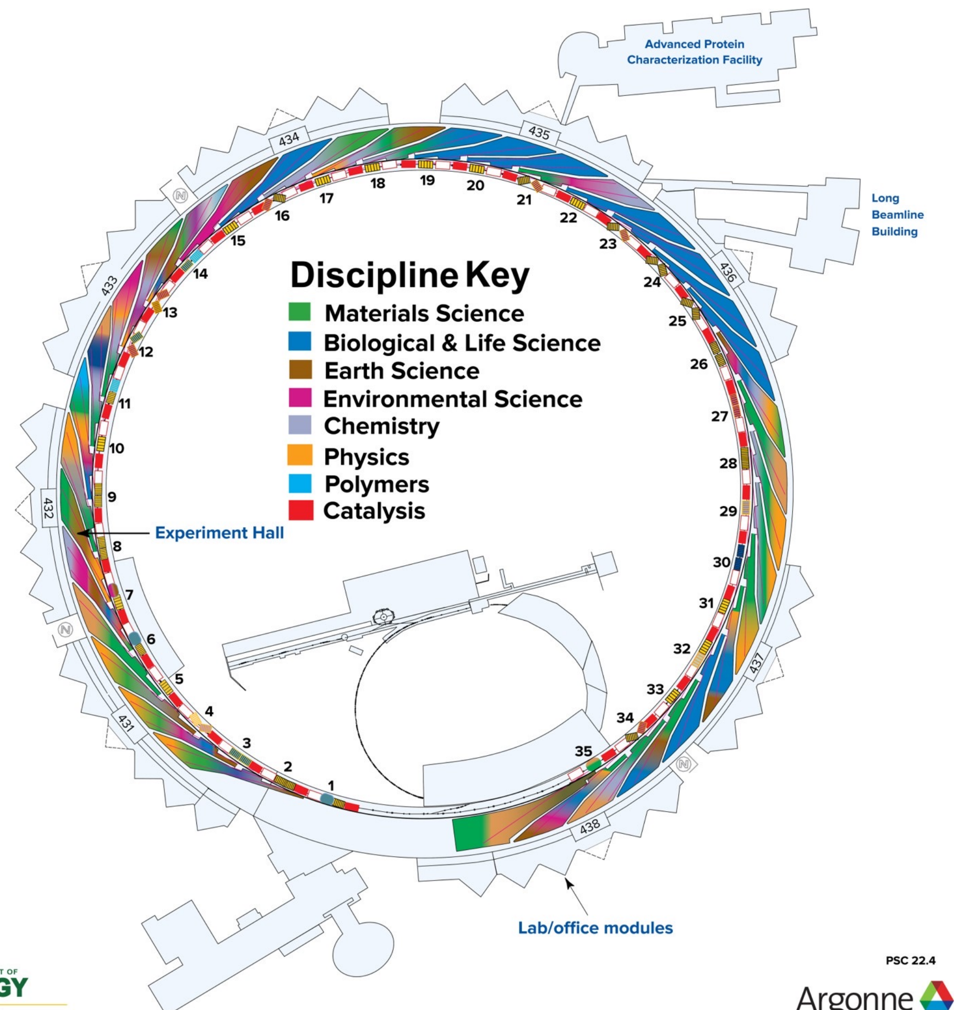
Beamlines:

67 beamlines, 47 ID, 20 BM

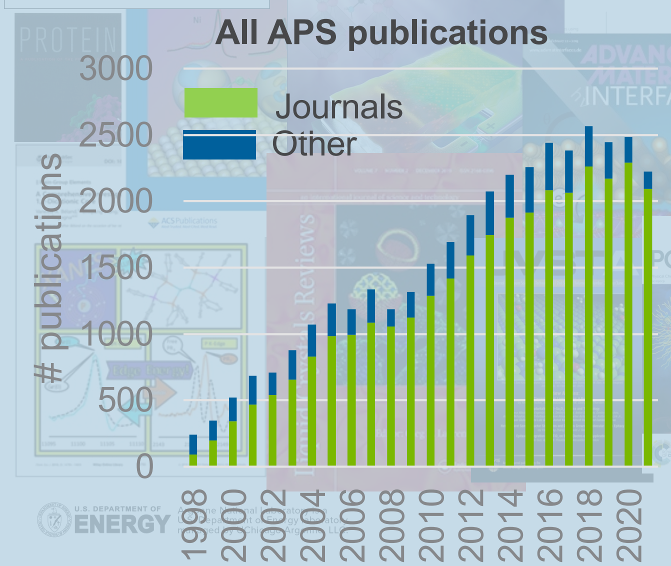
35 DOE-BES funded (base APS budget)

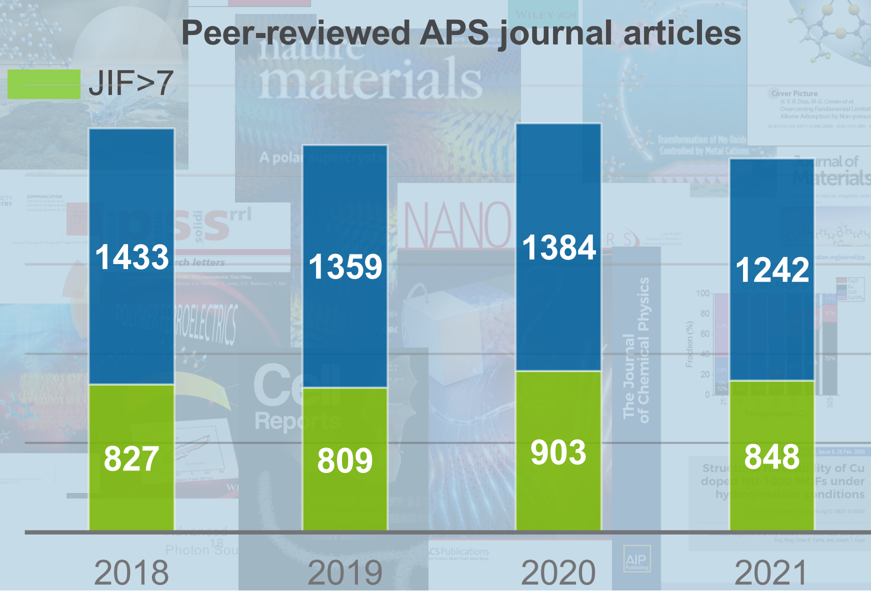
32 CATs (DOE-BER, NNSA, NIH, Industry)
8 APS operated

General user access via peer reviewed proposals



OUTPUT



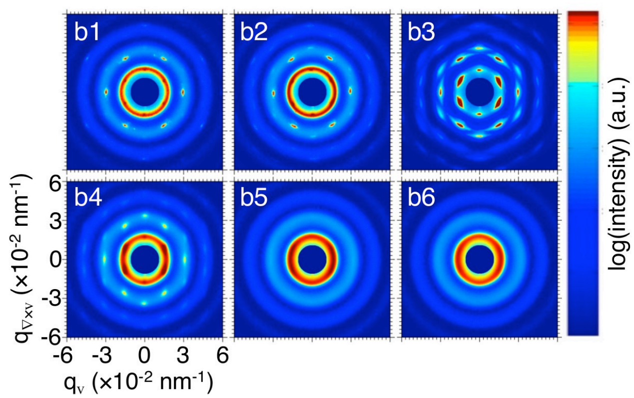


200 PhDs

APS BEAMLINES - SCATTERING

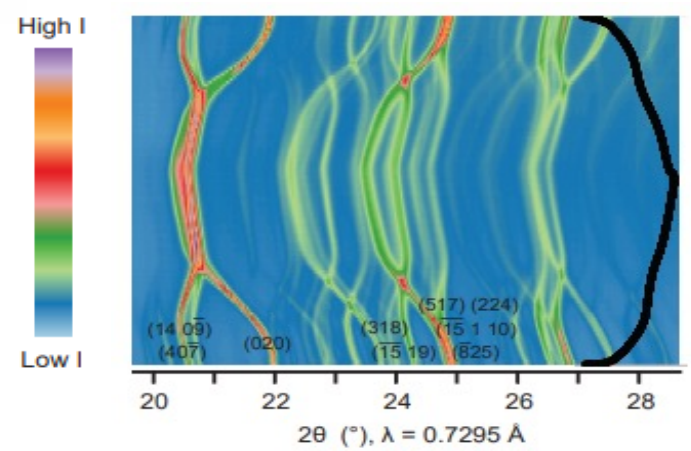
Structure of matter on length scales from atomic to µm.

- XRD, PDF
- SAXS/USAXS/WAXS
- High Energy Diffraction Microscopy
- Single Crystal Diffraction
- **Surface scattering (in-situ growth)**
- **Bragg - Coherent Diffractive Imaging**



Jonghun Lee *et al., Phys. Rev. Lett.* **120**, 028002 (2018)

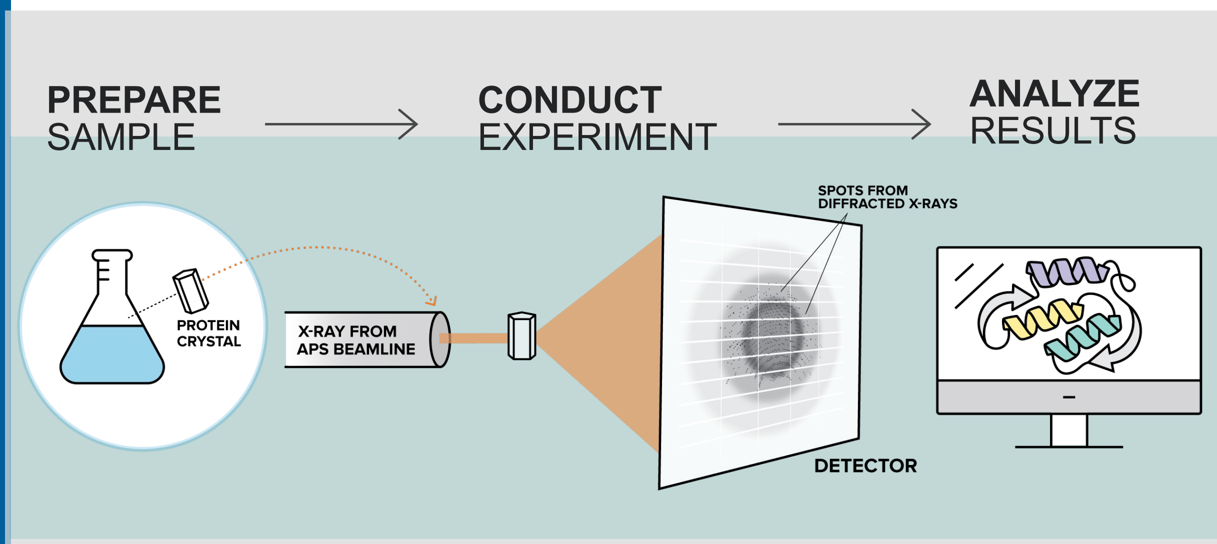
SAXS of colloids under shear

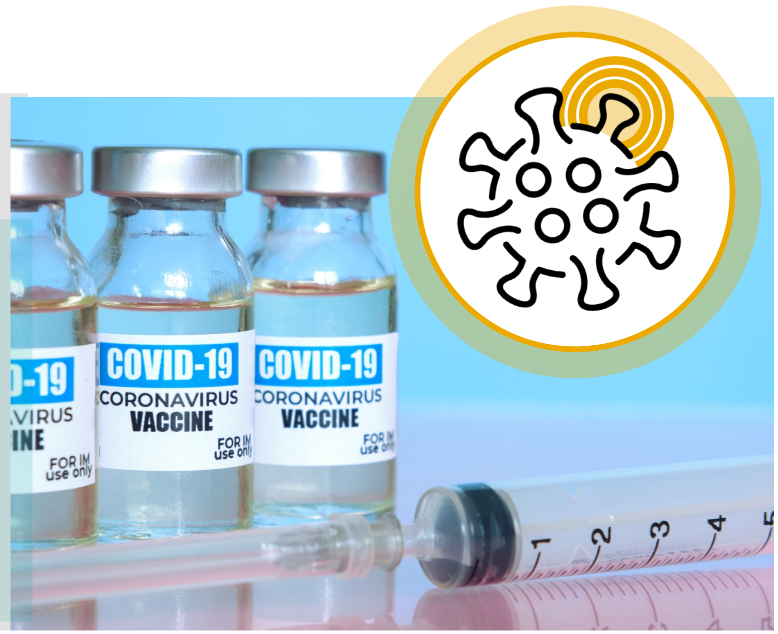


K. Griffin, et al., *Nature*, **559**, 556 (2020).

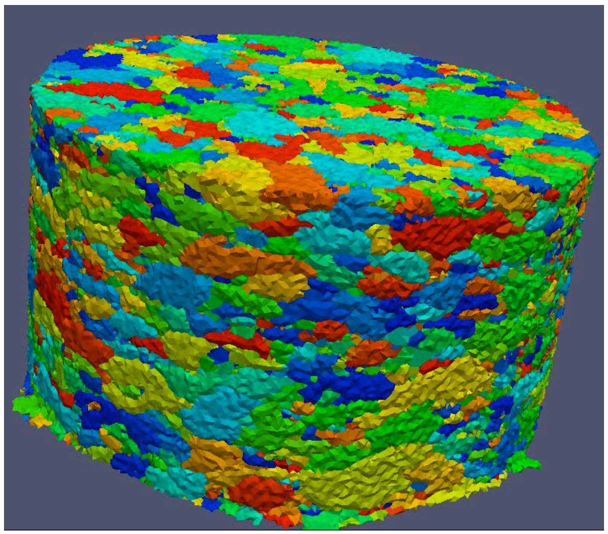
XRD of $Nb_{16}W_5O_{55}$ electrode

RESEARCH ON COVID

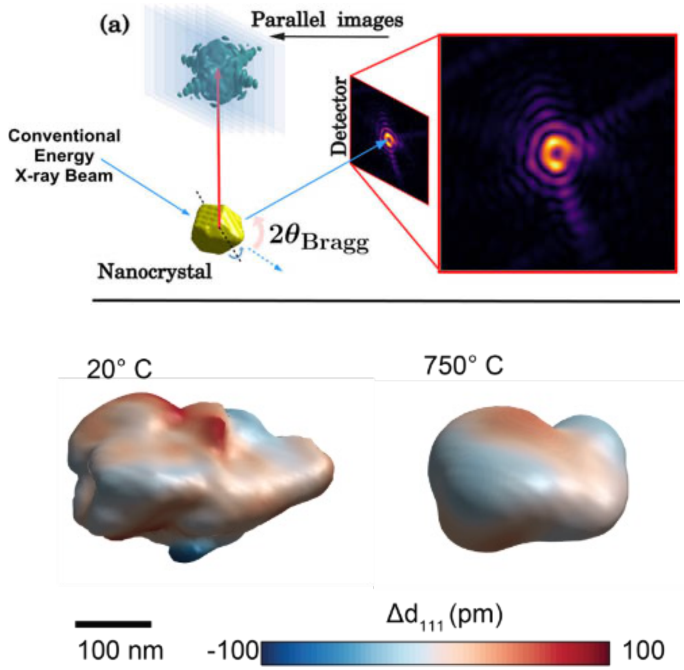




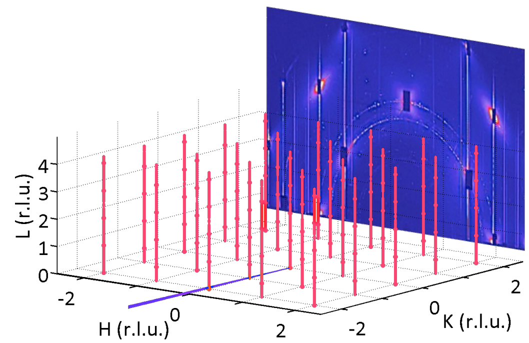
PROTEIN CRYSTALLOGRAPHY



HEDM of material under thermomechanical load



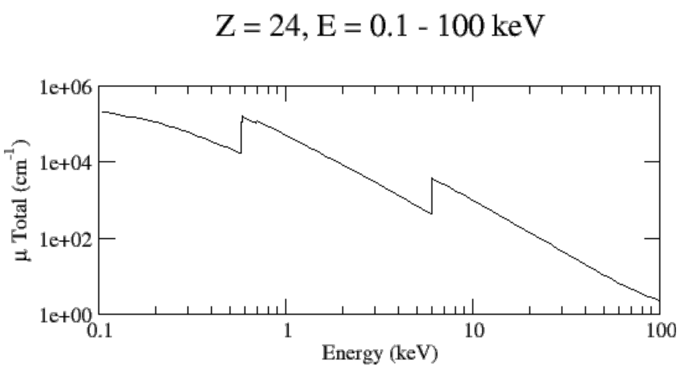
Bragg-CDI of diamond nanocrystals during annealing

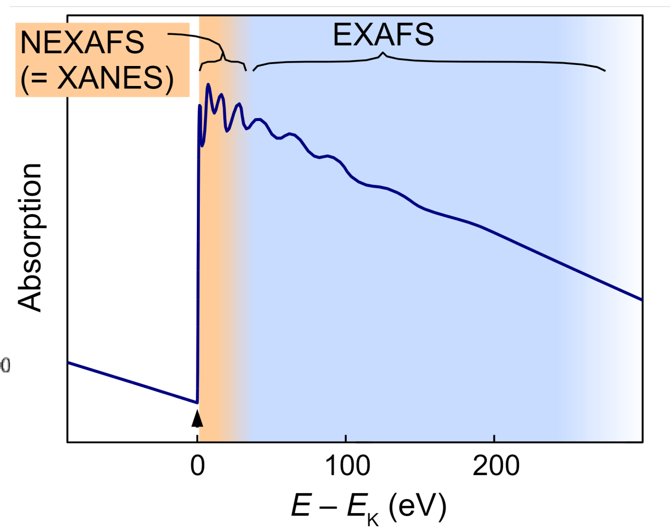


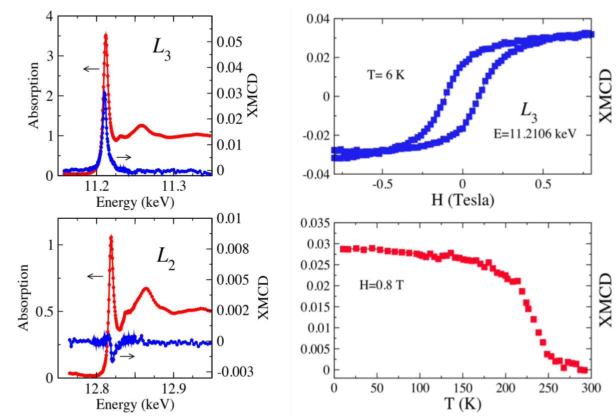
Coherent crystal truncation Bragg rods

SPECTROSCOPY

- XAS/ UltraFast-XAS, XMCD
- Nuclear Resonance Scattering
- **Inelastic Scattering, RIXS**
- **ARPES**



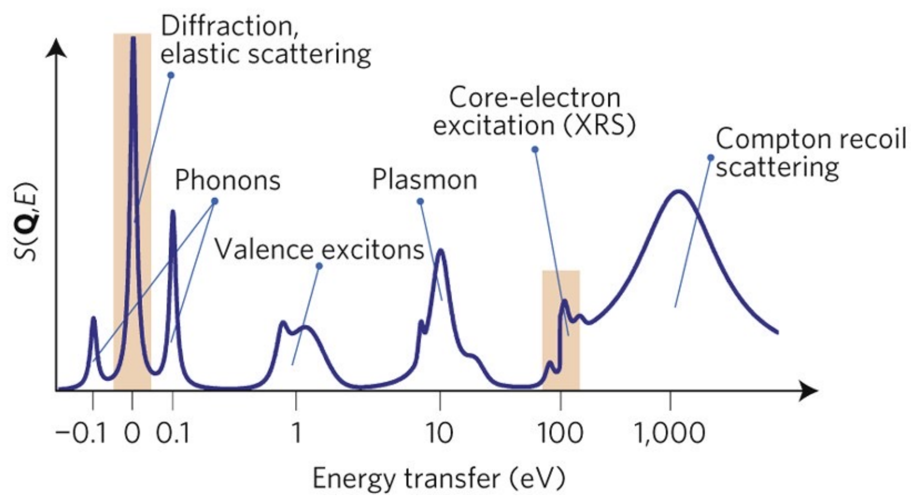




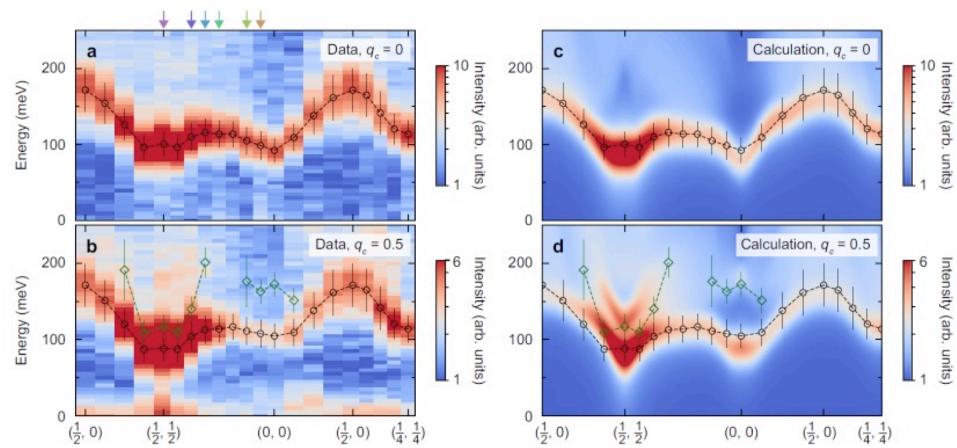
XMCD of Sr_2IrO_4

APS BEAMLINES - SPECTROSCOPY

Chemical, electronic, and magnetic states and dynamics (IXS) during reactions and applied external stimuli

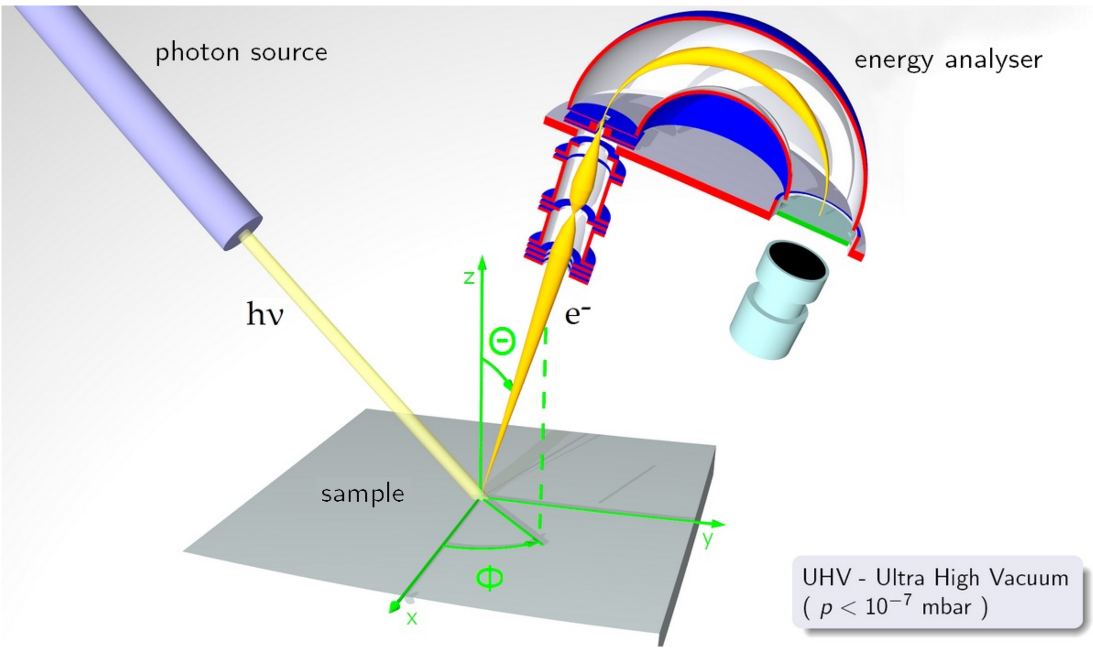


Huotari, S., Pylkkänen, T., Verbeni, R. et al. Direct tomography with chemical-bond contrast. Nature Mater ***10****, 489–493 (2011). https://doi.org/10.1038/nmat3031*

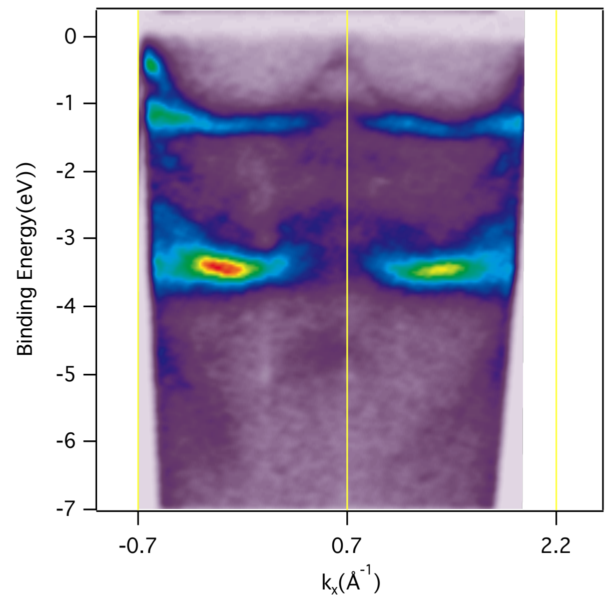


Mazzone, Det al. Nat Commun 13, 913 (2022)

APS BEAMLINES – ELECTRON SPECTROSCOPY

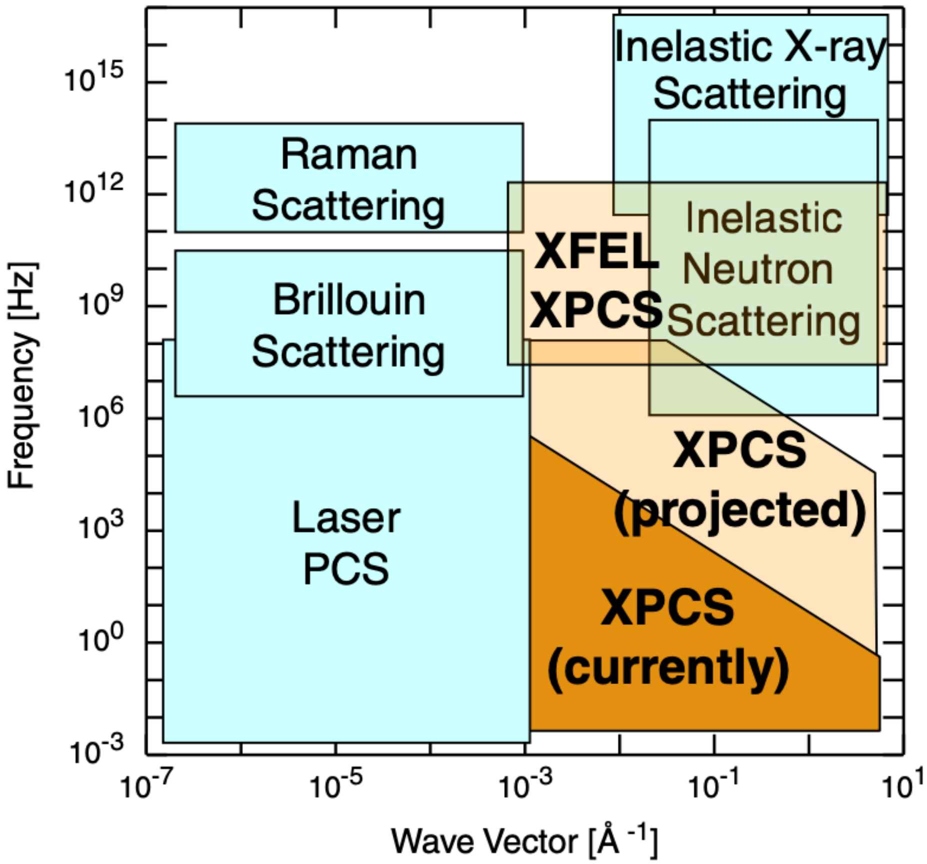


https://en.wikipedia.org/wiki/Angleresolved_photoemission_spectroscopy



ARPES of LaAlSi

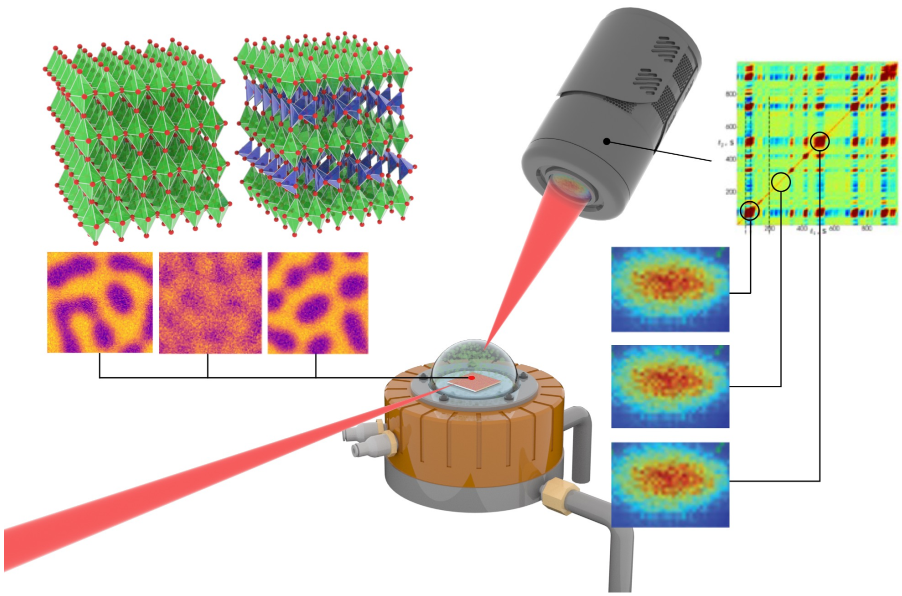
X-RAY PHOTON CORRELATION SPECTROSCOPY



- Dynamic structure factor probed in the time domain.
- Measuring speckle patterns at different time.
- Computing the intensity-intensity correlation function.

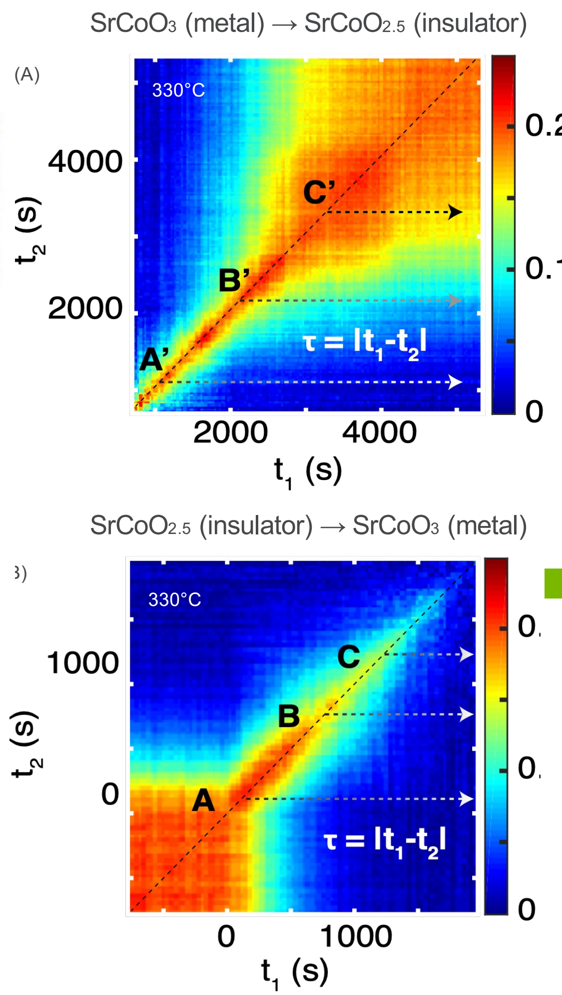
$$g_2(q,\tau) = \frac{\langle I(q,t)I(q,t+\tau)\rangle_t}{\langle I(q,t)\rangle_t}$$

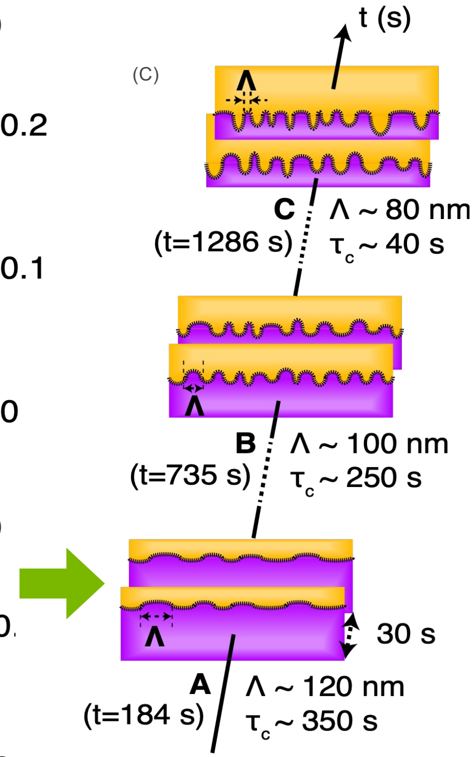
DYNAMICS DURING PHASE TRANSITION IN A RESISTIVE SWITCHING OXIDE



Research Detail

In situ redox, wide-angle XPCS measurements conducted at 8-ID-E in a complex oxide heterostructure



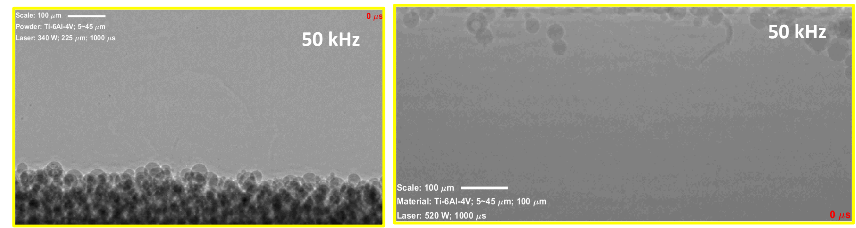


Two-time correlation function during reduction (A) and during oxidation (B) at 330°C. (C) Schematic demonstrating the dimensionality and dynamics of the oxidation process.

APS BEAMLINES - IMAGING

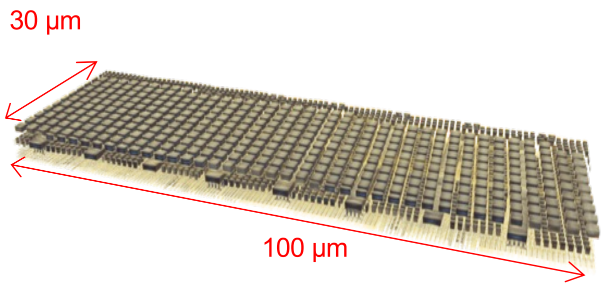
Dynamic (<ns to s) real space imaging with varying contrast (elemental, chemical, phase, …).

- Ultra-Fast Radiography (<1ns - ms)
- Rapid µ-Tomography (~1 µm)
- Transmission X-ray Microscope (~20 nm)
- Spectro-microscopy (20nm to µm)
- **Ptychography/Coherent Diffractive Imaging**



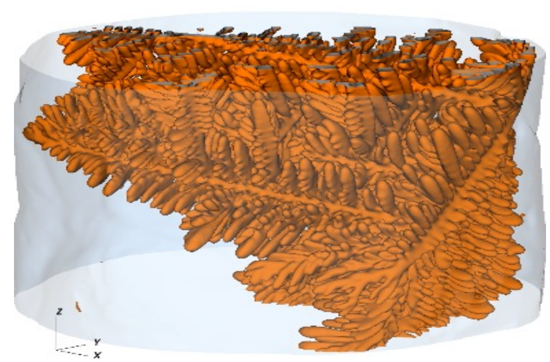
Cunningham *et al.*, *Science* **363**, 849 (2019)

In-Situ Radiography of laser powder-bed additive manufacturing



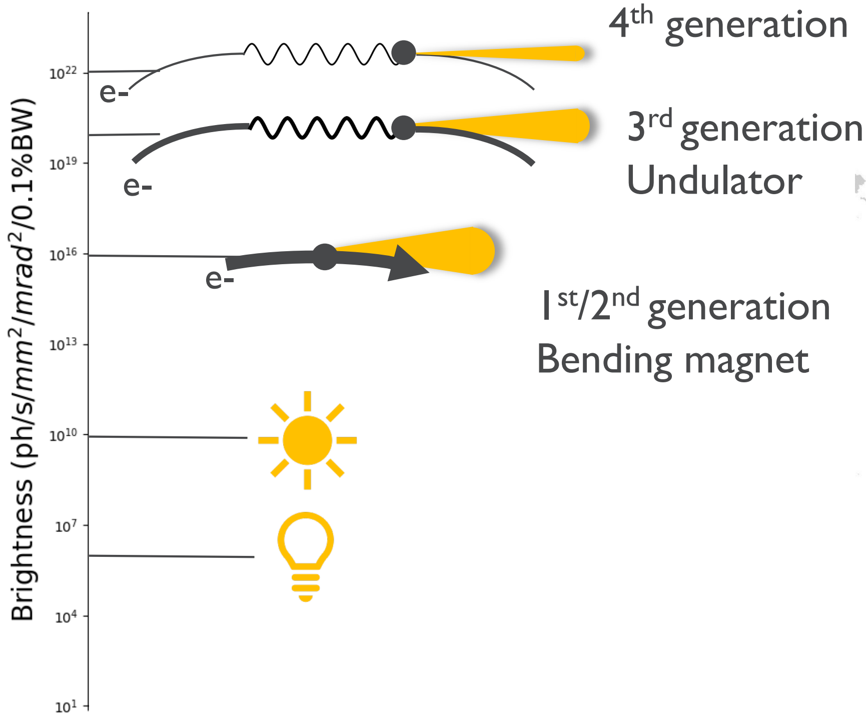
3D ptychography of an integrated circuit

Floures-Tomography of Zebra Fish



Rapid-Tomography of dendrite growth in aluminum

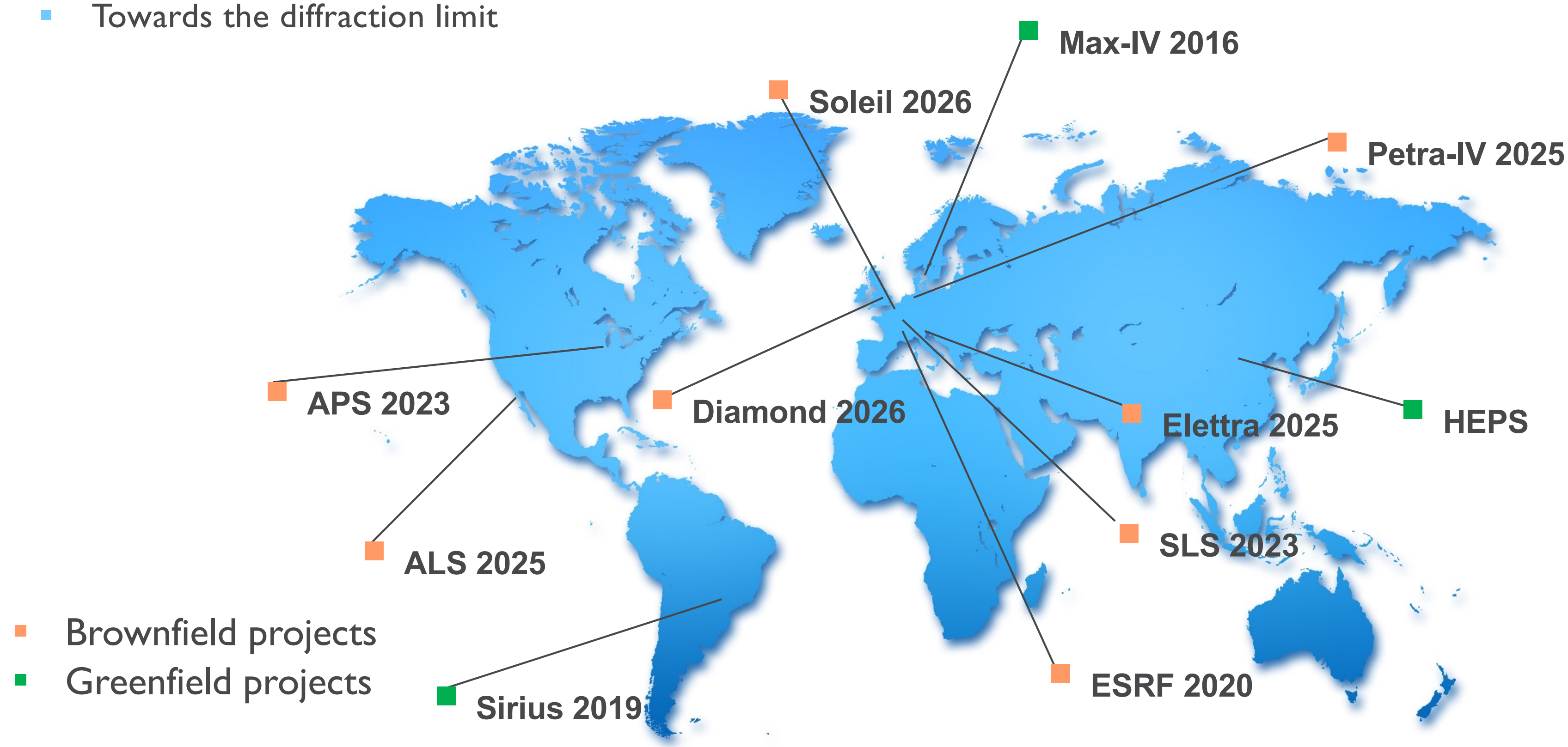
NEXT GENERATION SYNCHROTRON



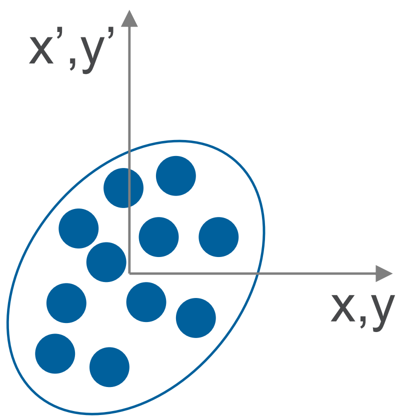
50 light-sources worldwide

4TH GENERATION PROJECTS

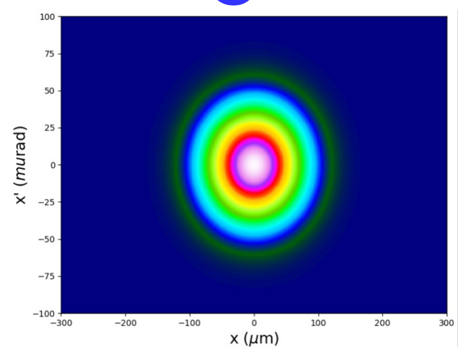
- 22 synchrotrons planning 4th generation
- APS will be the brightest hard X-ray synchrotron after APS-U delivery by 2024
- Towards the diffraction limit



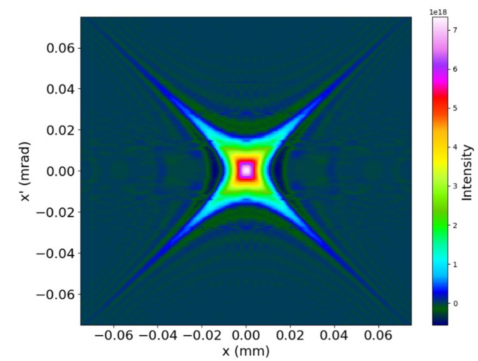
DIFFRACTION LIMITED STORAGE RING



e-



Undulator

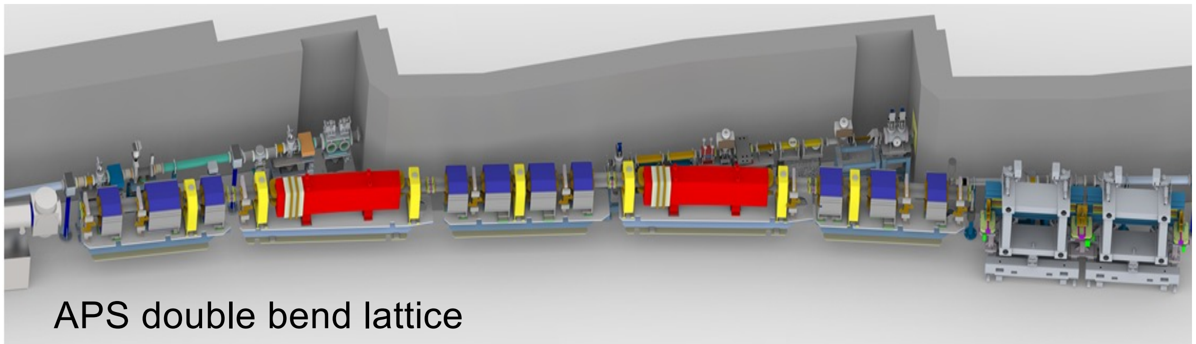


- Phase space distribution of an undulator is far from Gaussian
- However, fully coherent in the limit of zero electron beam emittance and zero energy spread
- Lower the electron emittance to make it negligeable compared to the natural emittance. Diffraction limited if :

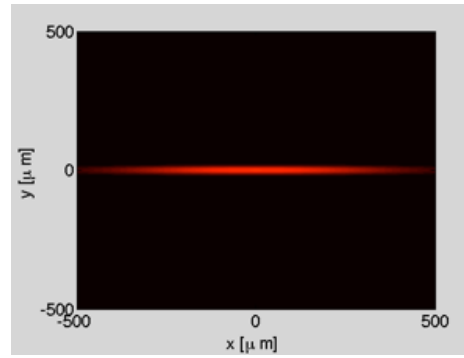
$\varepsilon_{x,y} \ll \frac{\lambda}{4\pi}$ (rms) $\varepsilon_{x,y} \ll \frac{\lambda}{2}$ (FHWM)

APS-U – HIGH BRIGHTNESS STORAGE RING LATTICE

APS Today

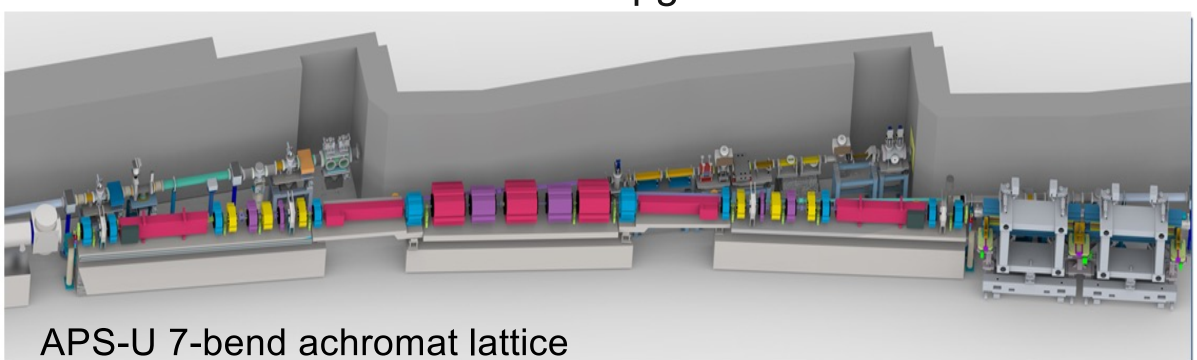

APS double bend lattice

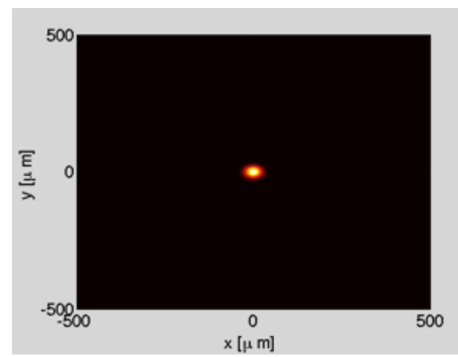
APS Today



ε_o = 3100 pm.rad

APS Upgrade


APS-U 7-bend achromat lattice



ε_o = 42 pm.rad

APS-U SECTOR

x500

$815M

$1.5B

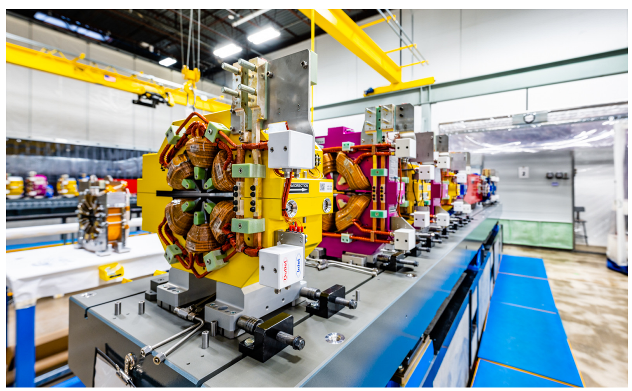

A new storage ring


New experimental facilities


New infrastructure, which will house two feature beamlines





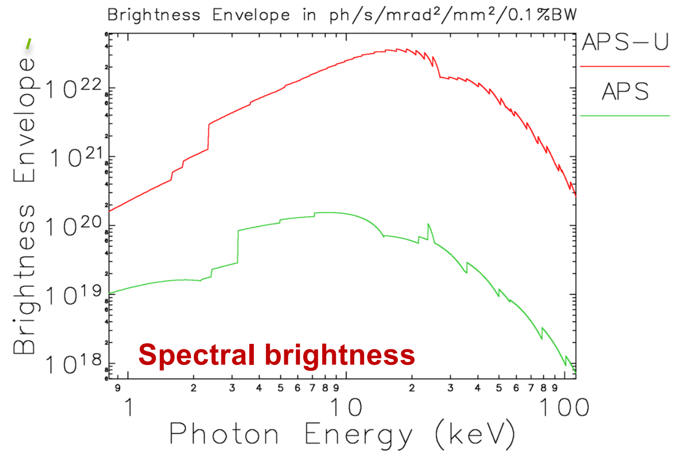


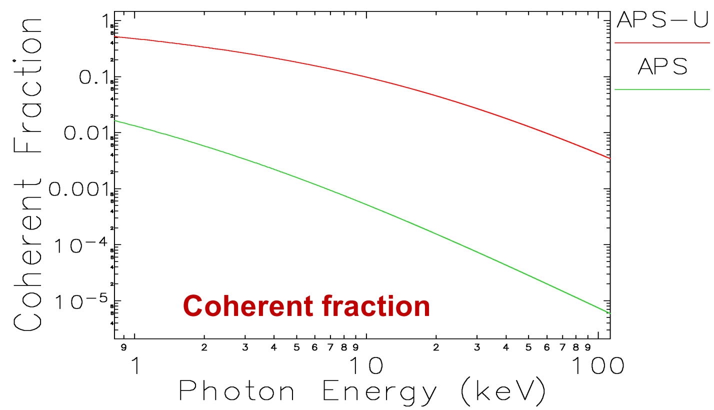

PROGRESS IN PICTURES

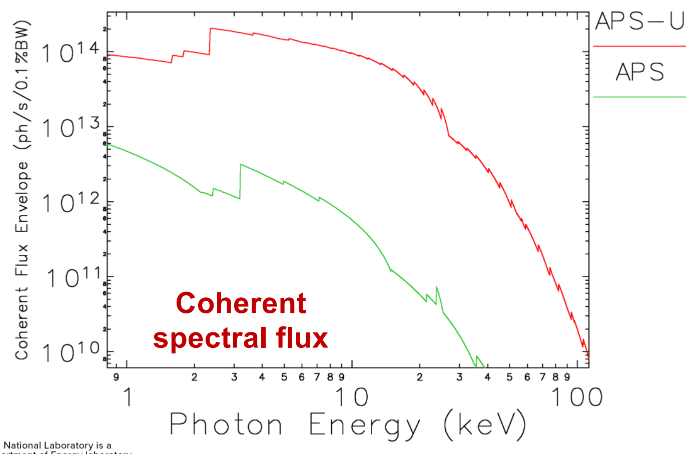
Storage Ring Enclosure, June 9

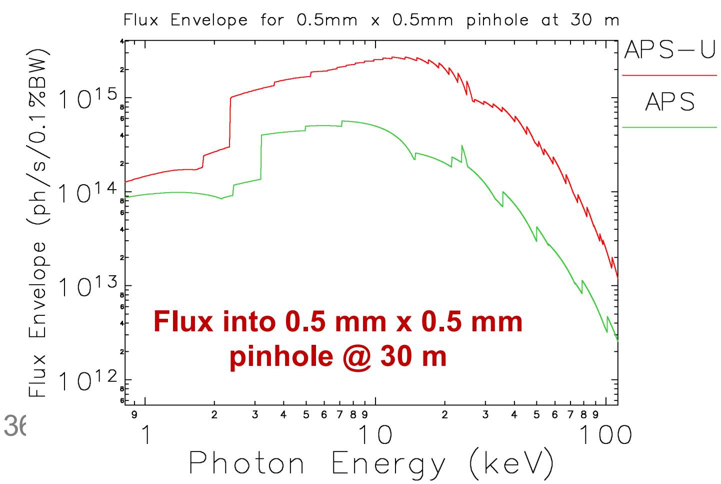
Sector 24 looking upstream, July 19

APS-U – HIGH BRIGHTNESS STORAGE RING LATTICE



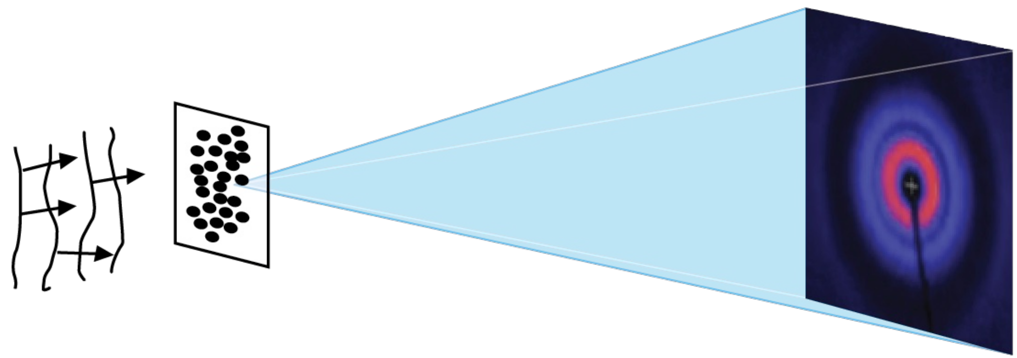




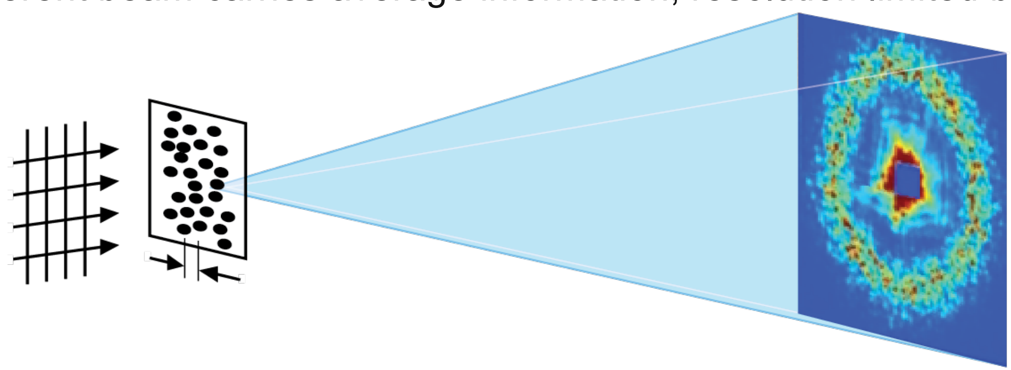


Coherent x-ray studies

Game-changing leap from average to local time/space information



Incoherent beam carries average information; resolution limited by optics



Scattering of coherent beam carries all microscopic, local information

non-periodic arrangements, correlations, dynamics

Spatial resolution limited only by x-ray wavelength, coherent flux

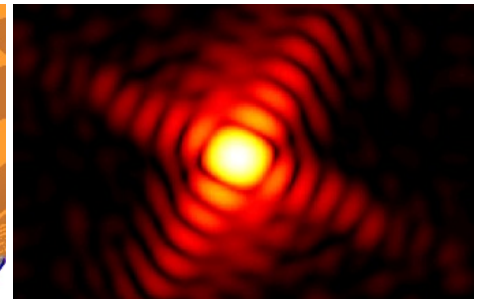
DRIVERS

HIGH ENERGY

Penetrate bulk materials and operating systems

BRIGHTNESS

Provide 3D fields of view, at a scale visible to the naked eye, with resolution at the nanometer scale



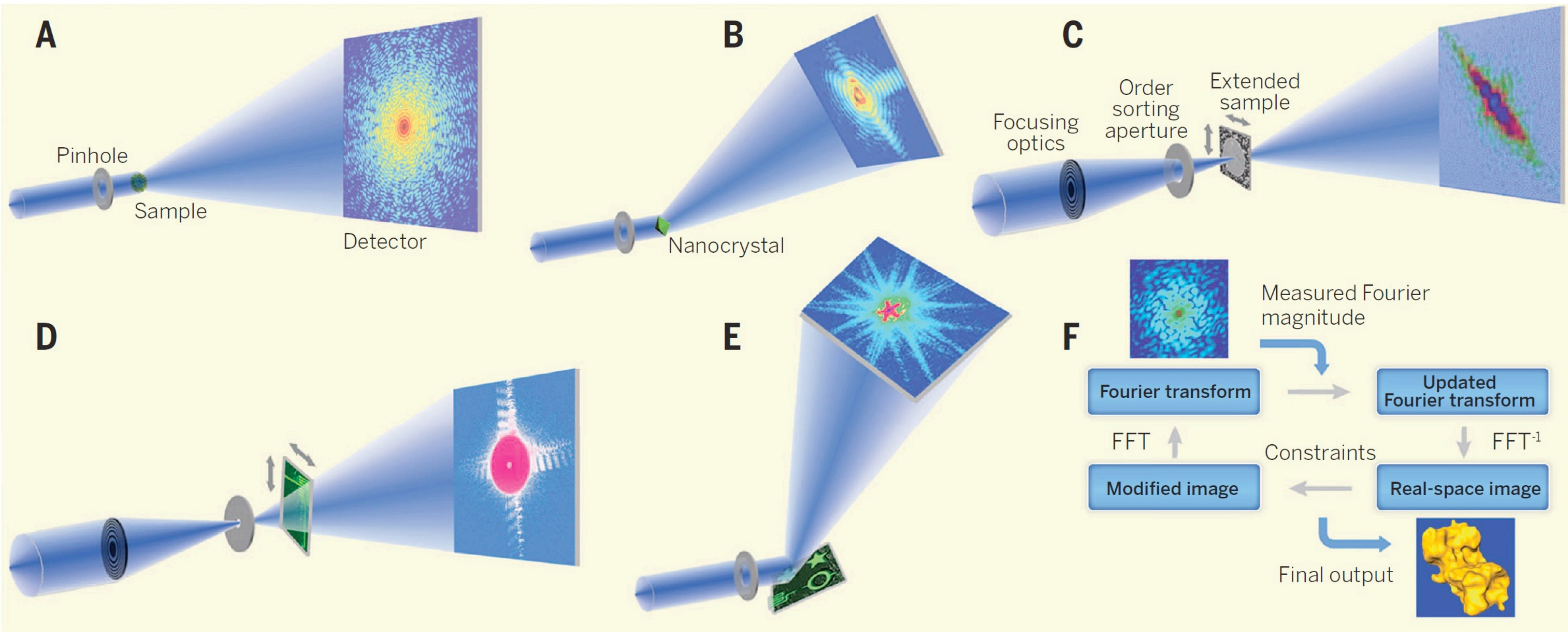
COHERENCE

Enable highest spatial resolution even in materials that do not have a fixed, repeating structure

DATA SCIENCES

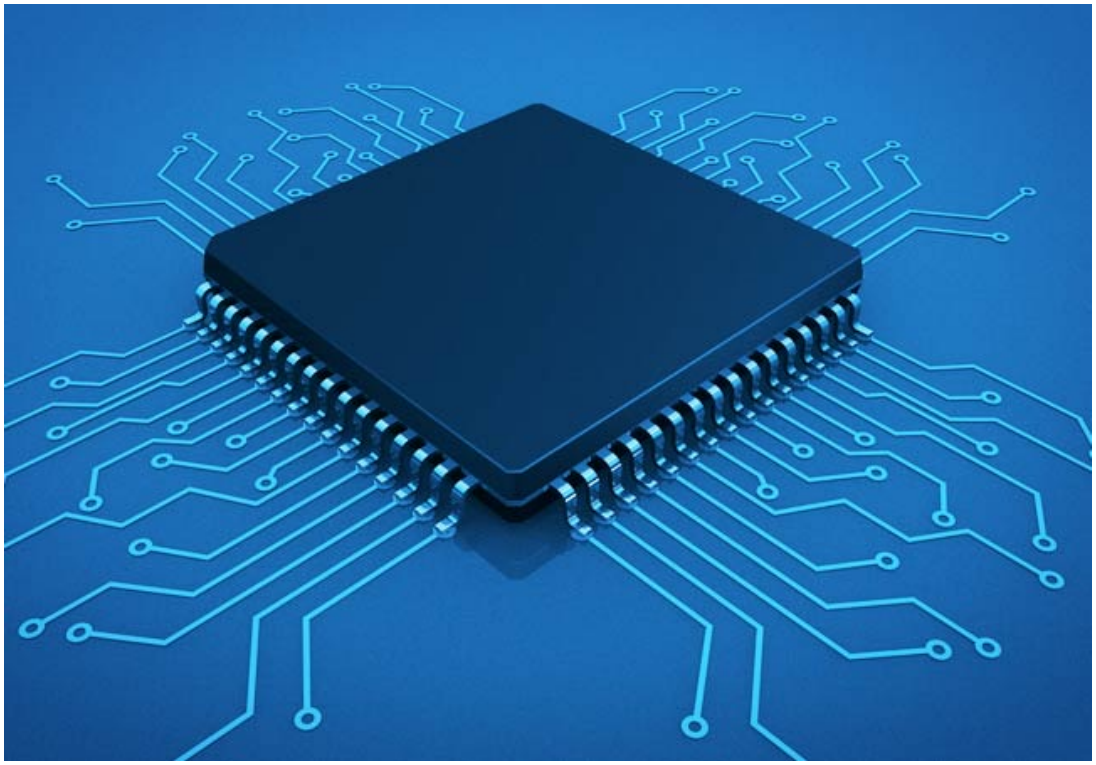
Enable real-time data analysis and decision making at the beamline

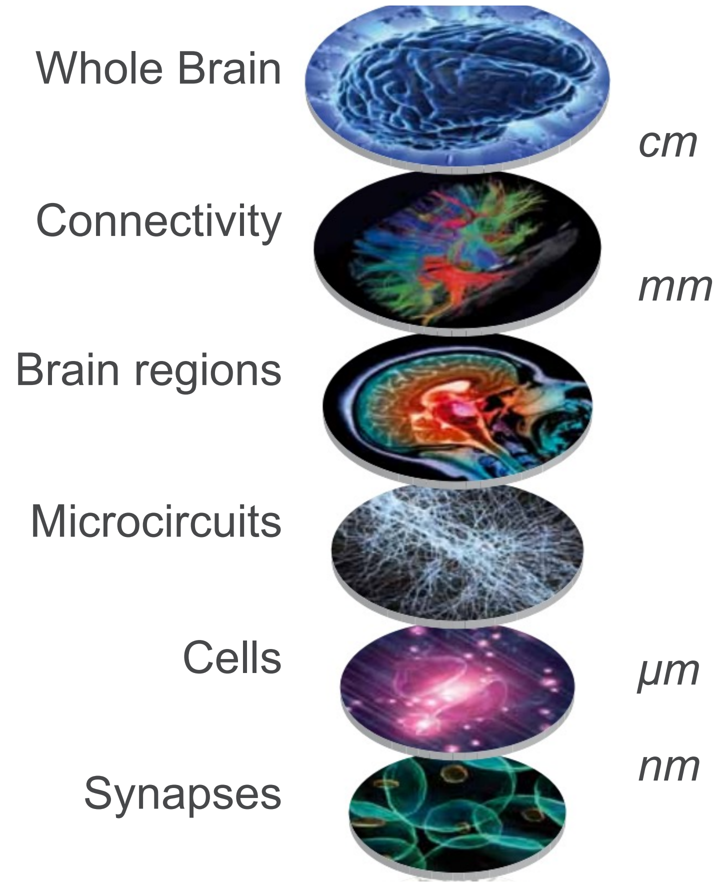
COHERENT DIFFRACTION IMAGING



Miao, Science, VOL 348 ISSUE 6234, (2015)

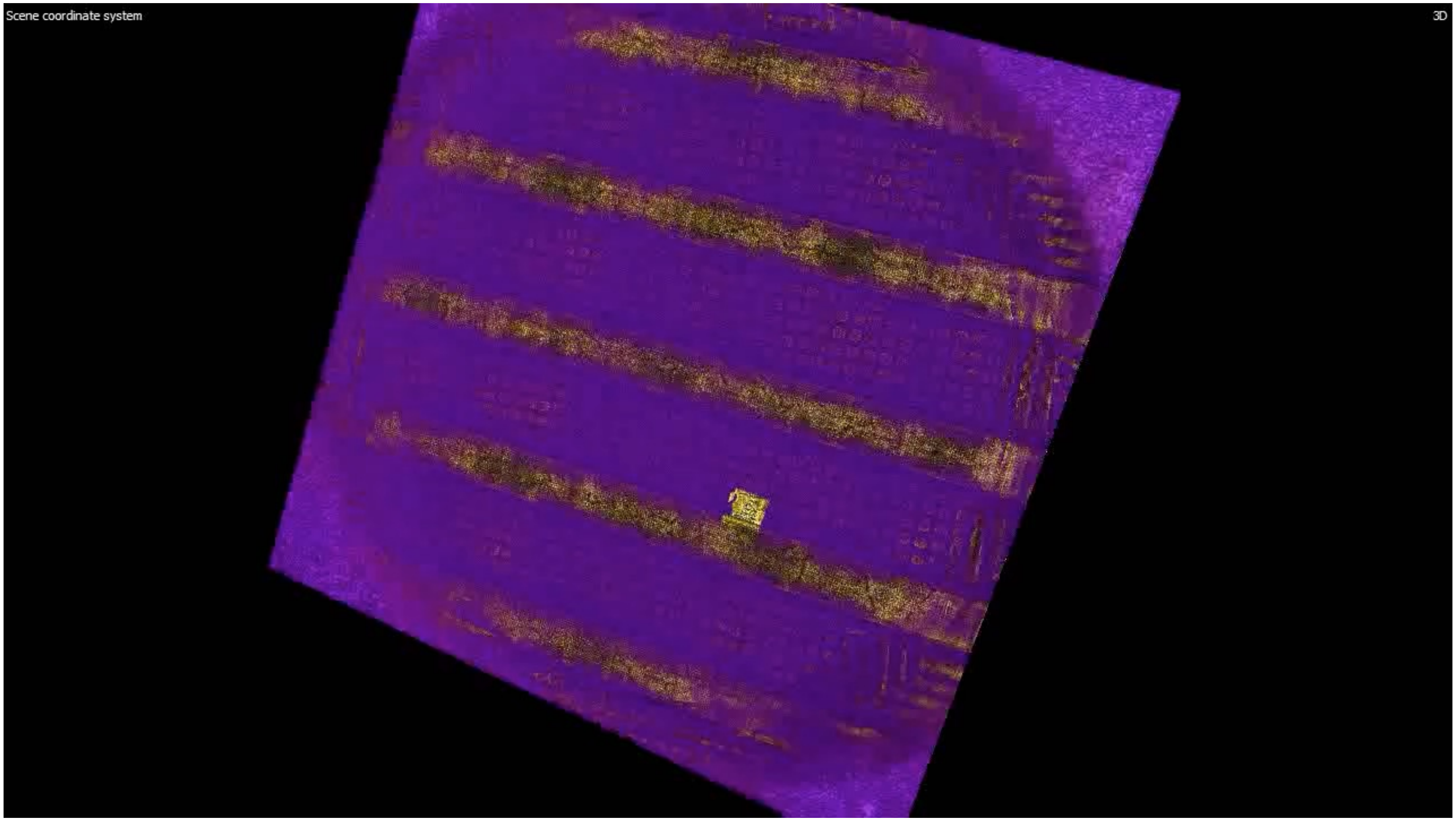
UNIQUE OPPORTUNITY: LENSLESS IMAGING OF EXTENDED 3D SAMPLES





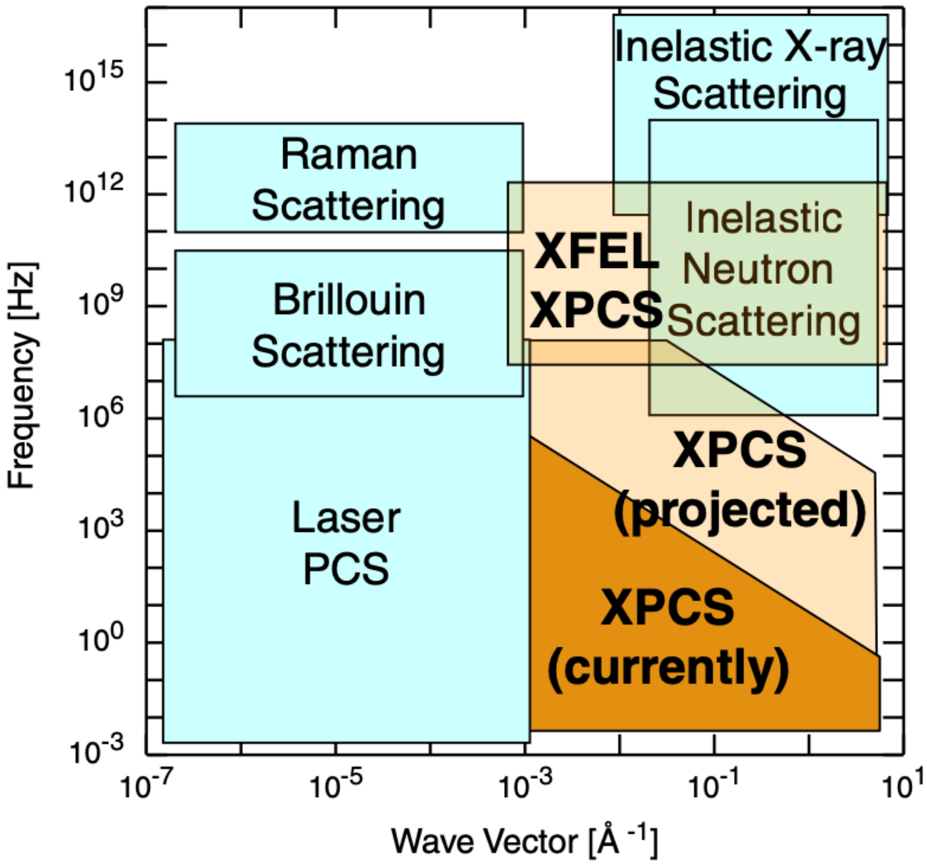
With APS-U: coherent flux to image $1 mm^3$ at 10 nm 3D resolution in ~1 day

LAMINOGRAPHY OF 16 NM IC



Scan FOV: 50 µm diameter

X-RAY PHOTON CORRELATION SPECTROSCOPY



- Dynamic structure factor probed in the time domain.
- Measuring speckle patterns at different time.
- Computing the intensity-intensity correlation function.

$$g_2(q,\tau) = \frac{\langle I(q,t)I(q,t+\tau)\rangle_t}{\langle I(q,t)\rangle_t}$$

Preparing for near-real-time science

The upgraded APS is expected to generate > 100 petabytes of data/year and will require up to 1 exaflop of peak computing power

100 petabytes/year
= 150,000 Netflix movies every day

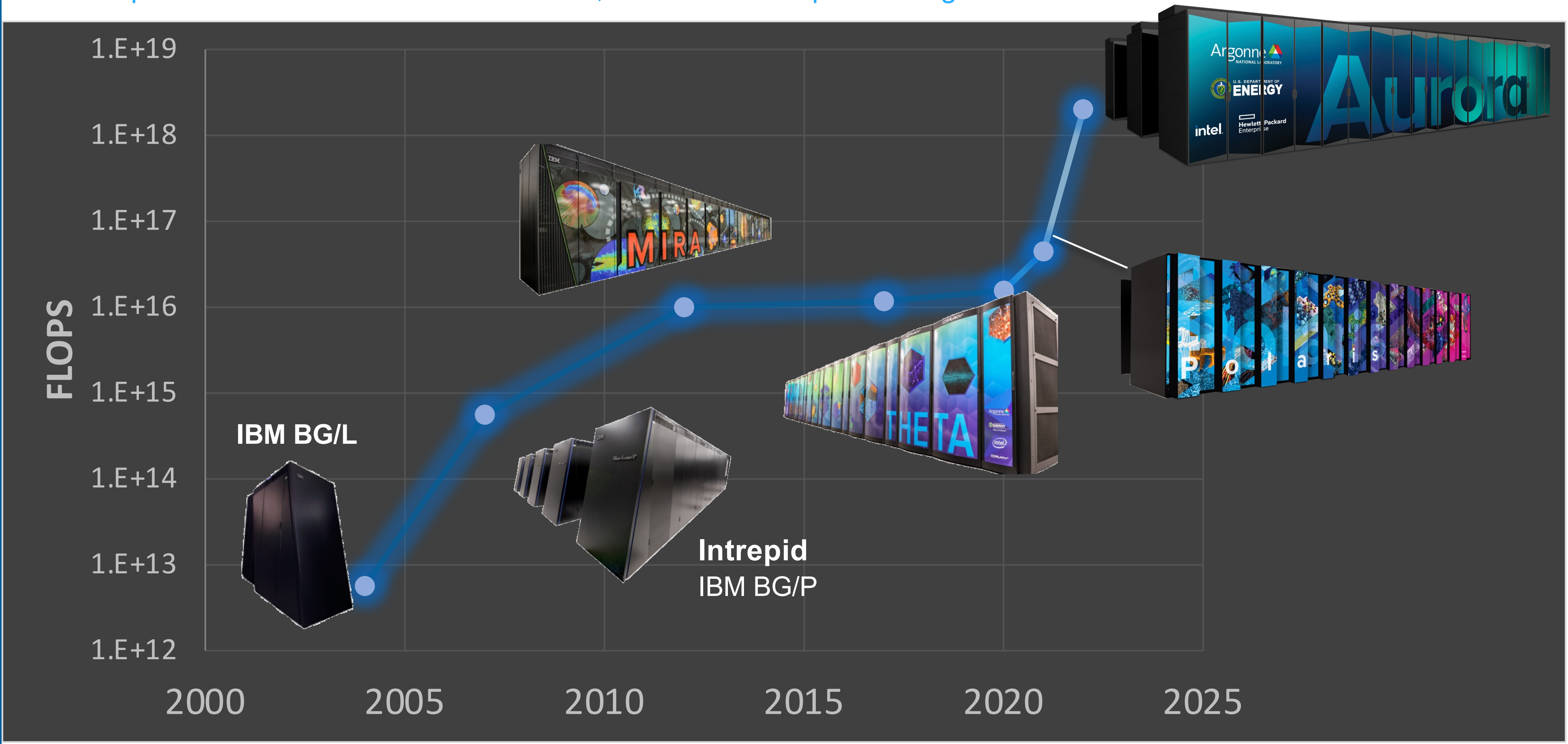
We need to look at every frame of every “movie,” analyze it in near real-time, and decide what to do

1 exaflop
= 500,000 servers

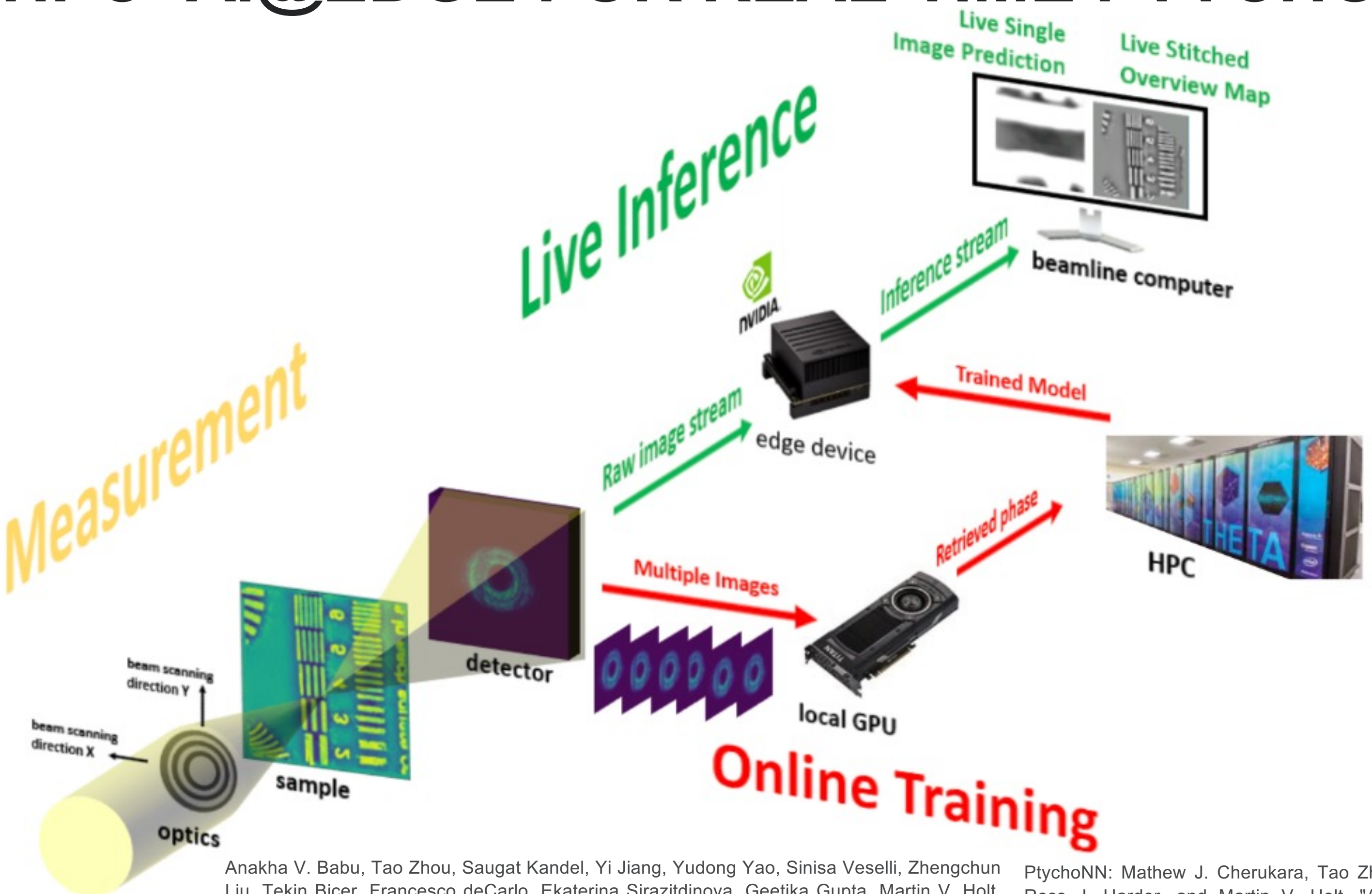
This will require ultrafast networks, archival storage, and a robust software infrastructure to support near-real-time analysis

The exascale era

New capabilities at exascale for simulation, real time data processing and reconstruction



HPC+AI@EDGE FOR REAL-TIME PTYCHOGRAPHY



- >100X faster
- Live inference @ 100 Hz on 512x512 images
- <25 X lower-dose imaging:

Anakha V. Babu, Tao Zhou, Saugat Kandel, Yi Jiang, Yudong Yao, Sinisa Veselli, Zhengchun Liu, Tekin Bicer, Francesco deCarlo, Ekaterina Sirazitdinova, Geetika Gupta, Martin V. Holt, Antonino Miceli and Mathew J. Cherukara, “Real-time nanoscale ptychographic X-ray imaging using deep learning at the edge”

PtychoNN: Mathew J. Cherukara, Tao Zhou, Youssef Nashed, Pablo Enfedaque, Alex Hexemer, Ross J. Harder, and Martin V. Holt. "AI-enabled high-resolution scanning coherent diffraction imaging." *Applied Physics Letters* 117, no. 4 (2020): 044103.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