Report on the Advanced Photon Source

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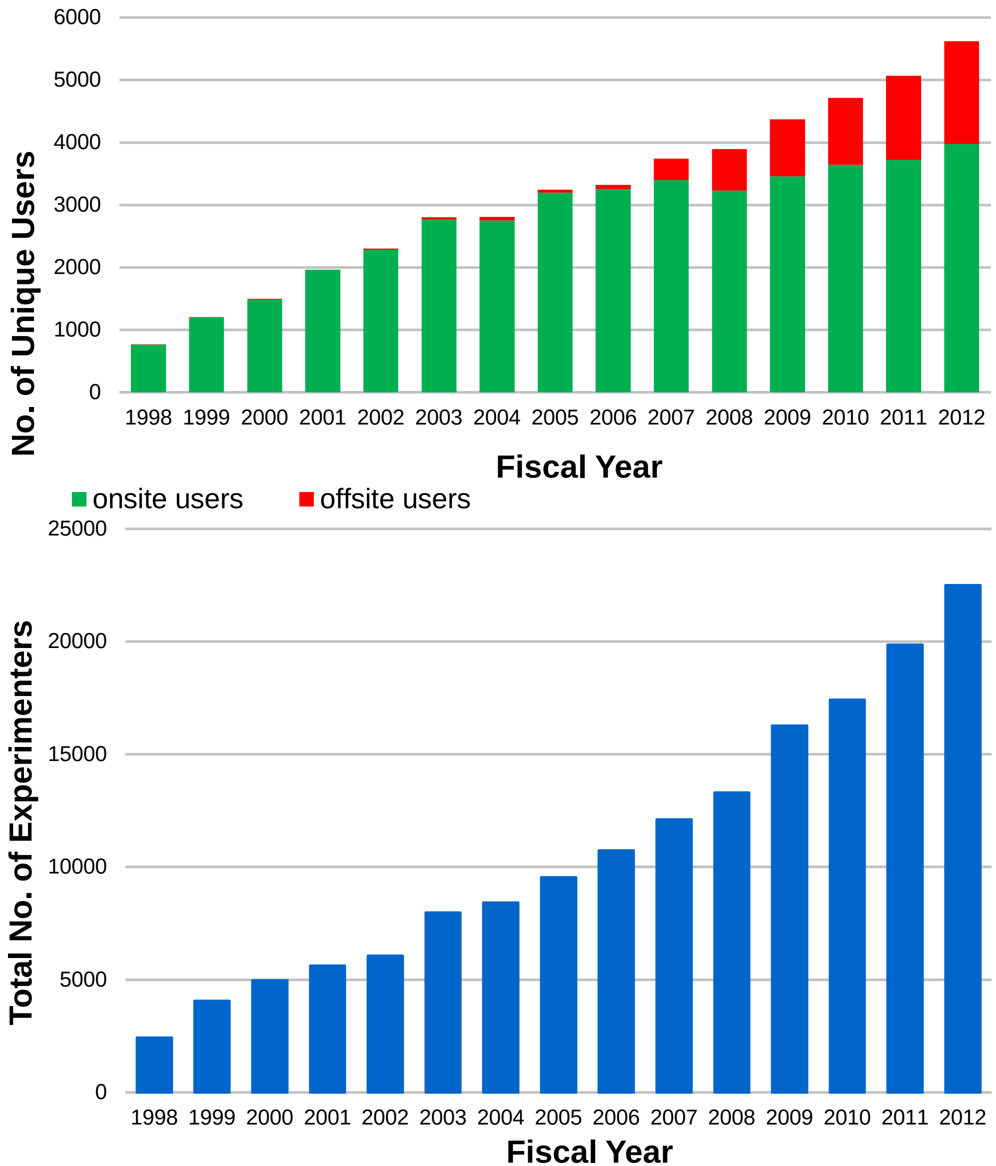
Argonne National Laboratory

Three-Way Meeting
August 1-2, 2013, Argonne

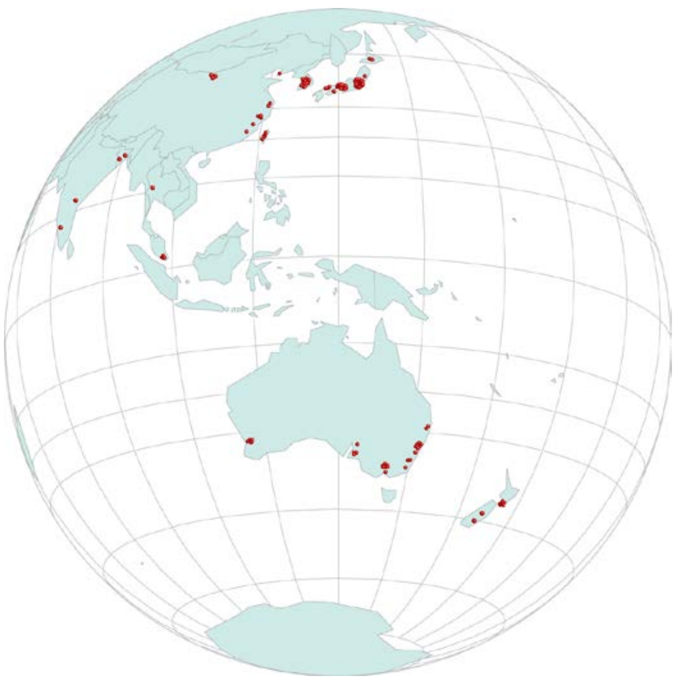
Advanced Photon Source in 2013

- 66 simultaneously operating beamlines, 5000 hours per year
- 22,500 participations by 5600 unique onsite and offsite users in FY12
- 4800 experiments in FY12
- 1550 total publications in CY2012, 20% high impact
- 1600 protein structure deposits per year, plus drug discovery programs
- Industrial users from 150 companies in pharma, energy, electronics, materials ...



APS Users FY 2012

APS user institutions in every U.S. state and worldwide



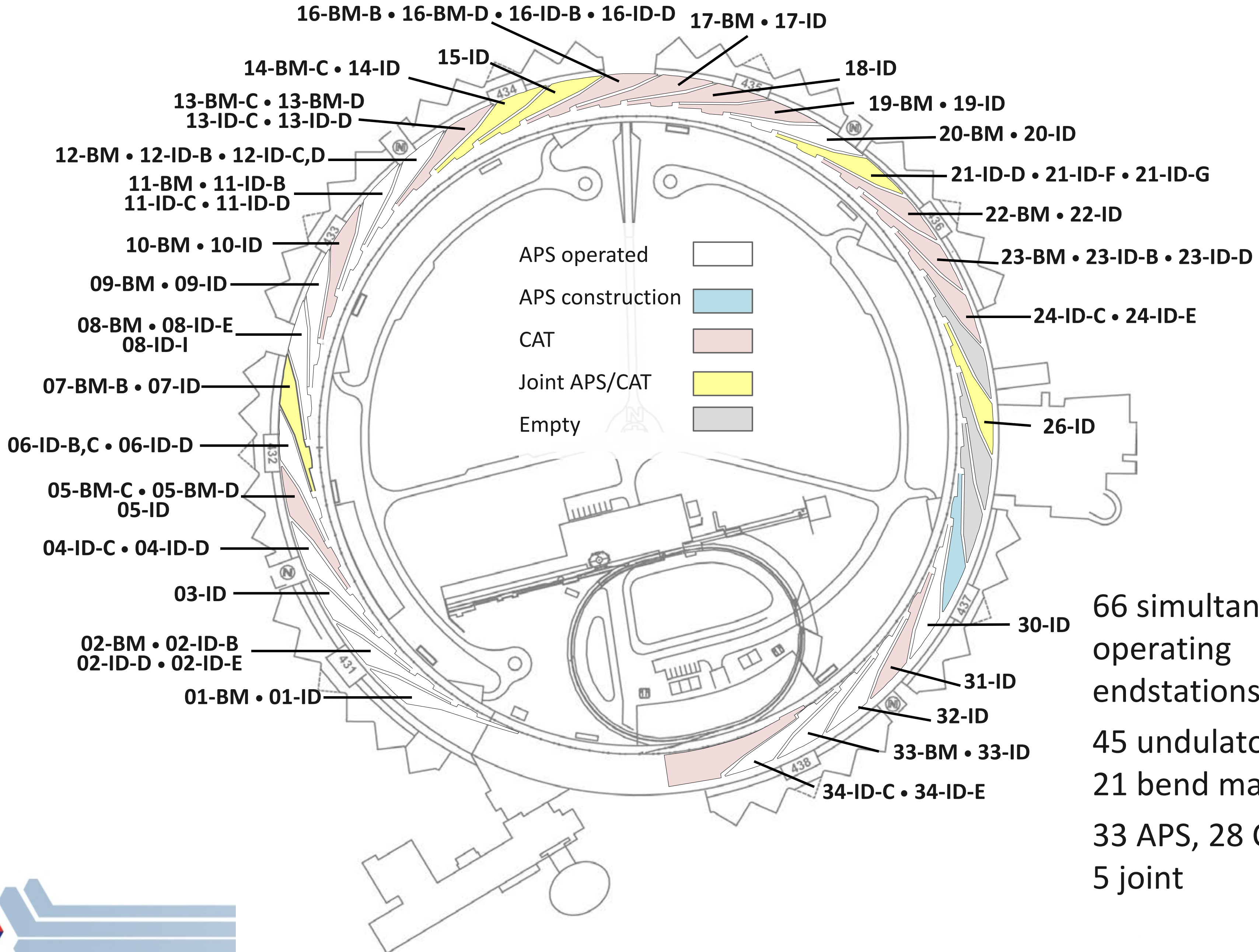
~1550 total publications in CY 2012

~5600 unique users in FY 2012

~4800 experiments in FY 2012

3

APS Beamline Layout 2013

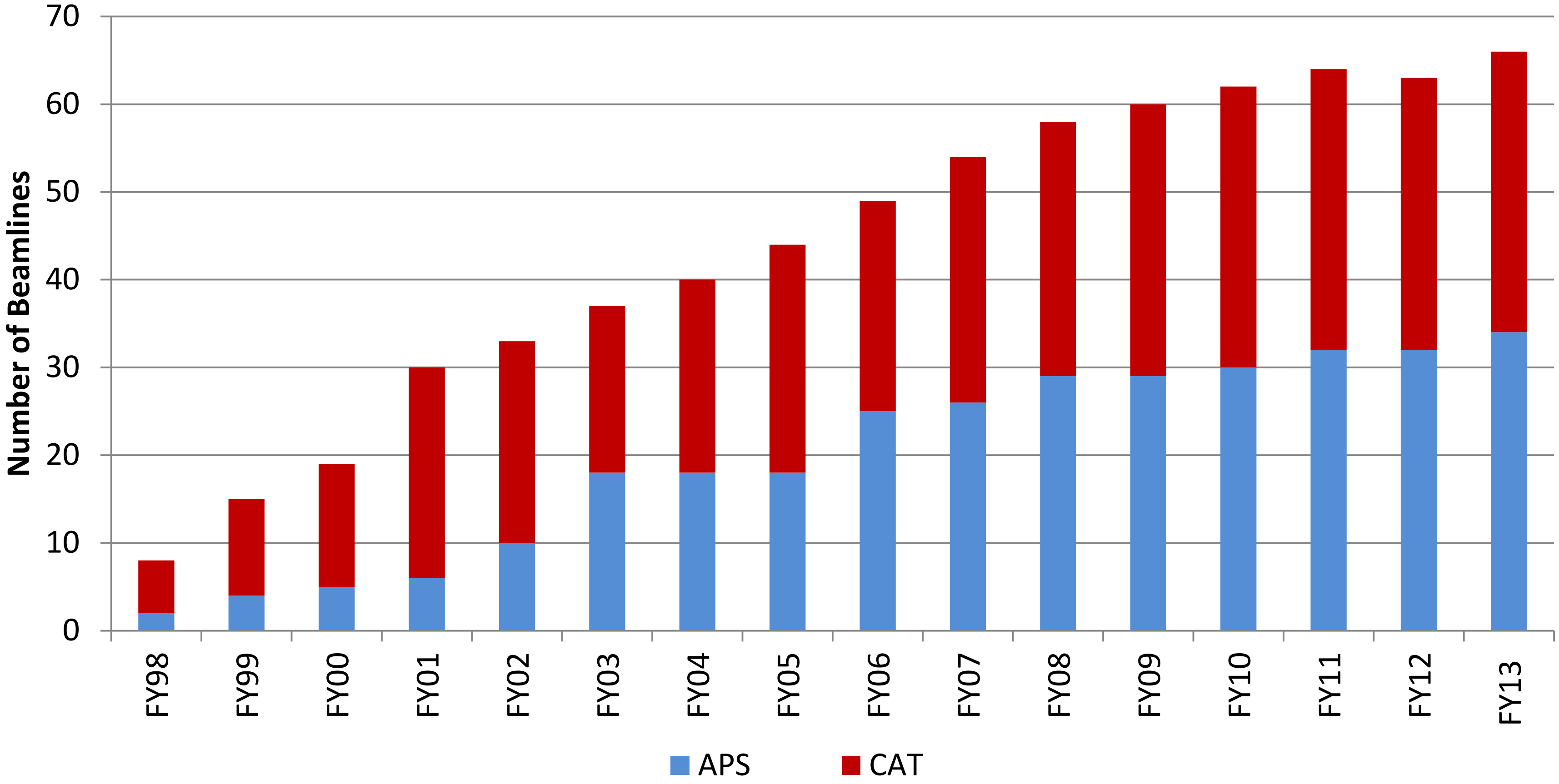


66 simultaneous operating endstations

45 undulator, 21 bend mag.

33 APS, 28 CAT, 5 joint

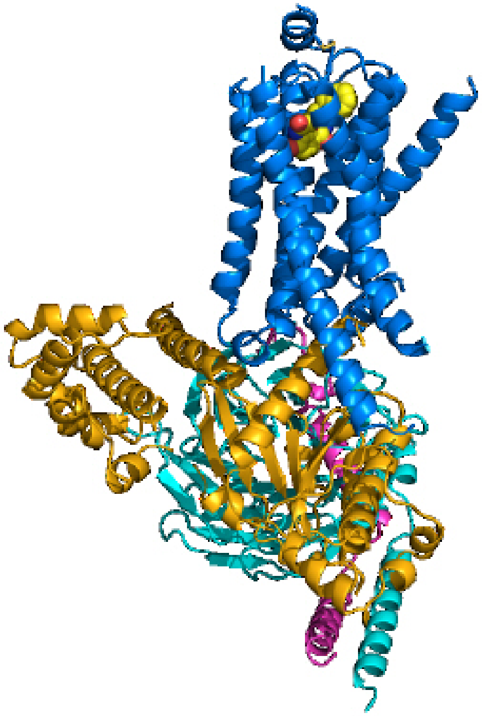
Strong Participation by Collaborative Access Teams (CATs) in Building and Operating Beamlines



The 2012 Nobel Prize in Chemistry to APS Researcher

- 2012 Nobel Prize in Chemistry awarded to Brian Kobilka (Stanford U., left above) and Robert Lefkowitz (HHMI, Duke U.) for work on G-protein-coupled receptors (GPCRs)
- 2011 study by Kobilka et al. at APS Sector 23 provided the first high-resolution look at transmembrane signaling by GPCR
- Added critical insight about signal transduction across the plasma membrane, a discovery the Nobel announcement deemed “The Holy Grail, a high-resolution structure of an active ternary complex”

S.G.F. Rasmussen et al., Nature **477**, 549 (29 September 2011) DOI:10.1038/nature10361



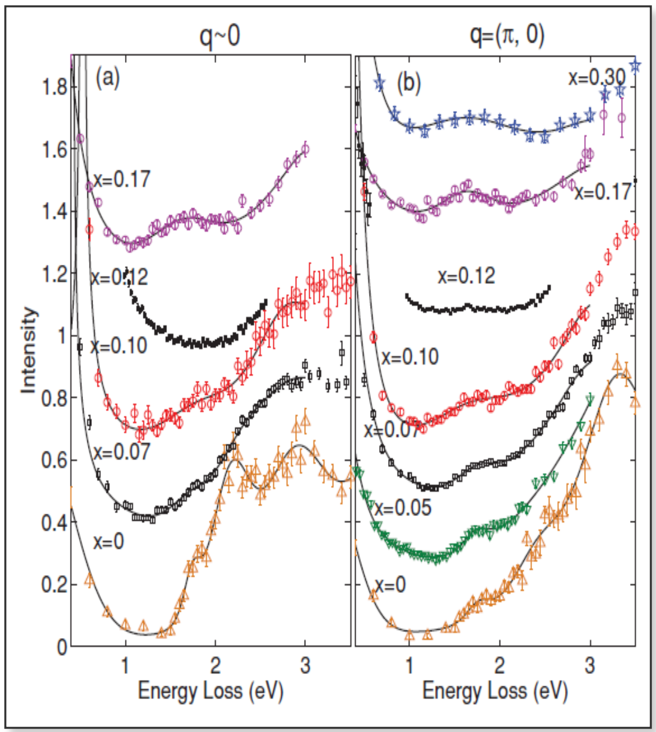
The structure of the β_2AR-Gs complex

Transforming study of the origins of excitations in strongly correlated electrons

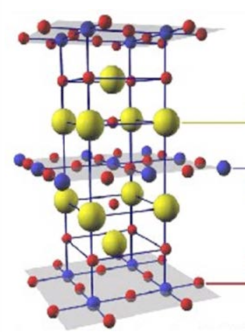
How do delicate low-energy phenomena emerge from Coulomb forces at eV-scales?

Current Capability

- Resonant Inelastic X-ray Scattering – dynamic structure factor, S(**q**,ω)



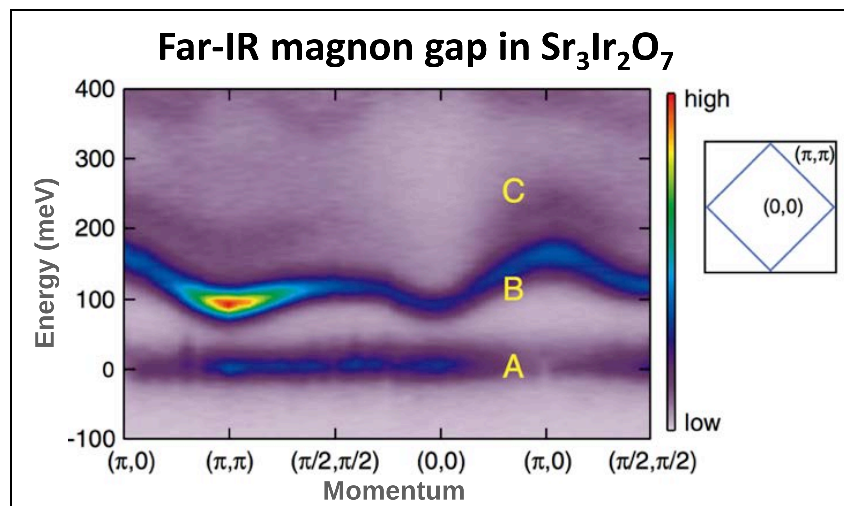
D. S. Ellis, et al., Phys. Rev. B ***83****, 075120 (2011)*



$La_{2-x}Sr_xCuO_4$

Capability with APS-U

- APS-U will transform study of mid- to far-IR electronic & magnetic excitations
- New RIXS spectrometer with orders-of-magnitude increase in signal enables S(**q**,ω) 'sum rule' measurements
  - 300x at 20 meV



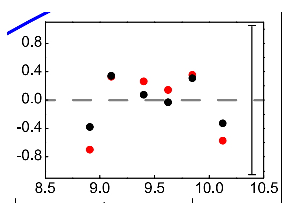
J. Kim, et al., Phys. Rev. Lett. ***109****, 157402 (2012)*

High pressure: Expanding the frontiers of experimental science

Can we use high pressure to understand planetary cores and discover new states of matter?

Current Capability

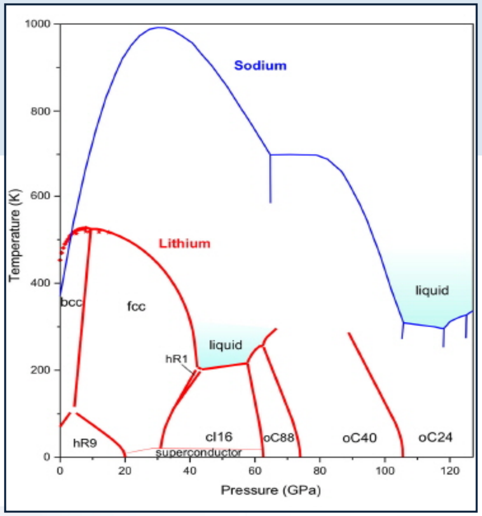
- X-ray techniques combined with high-pressure cells reveal myriad impacts of pressure on atomic/molecular interactions
  – Diamond anvil cell used for spectroscopy study of Fe at elevated T's and P < 280 GPa



Determining properties of earth's core: *Vp –ρ* of hcp-Fe and hcp-$Fe_{0.85}Si_{0.15}$ at high pressures and temperatures. Findings indicate significant *Vp –ρ* differences that call for addition of ~8–10 wt % light elements in outer core and 4 wt % in inner core (e.g., 12–15, 23); *Z. Mao et al., PNAS USA* ***109****, 10239-10244 (2012)*

Capability with APS-U

- Higher brightness, smaller spot sizes enable use of full array of x-ray techniques at new range of pressures
  – Multi-Mbar conditions allowing studies beyond planetary core pressures of > 350 GPa
  – Creating new states of matter



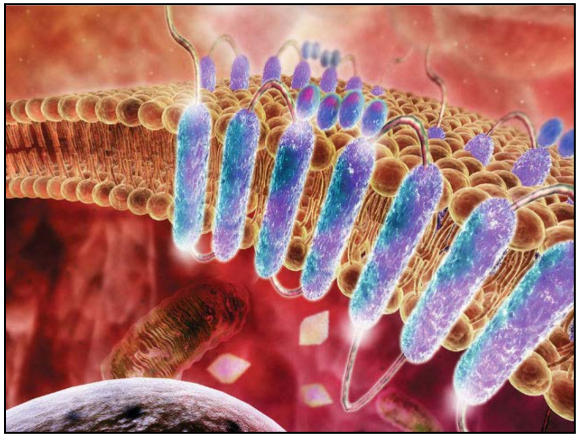
Zero point motion: Enhanced quantum effects in simple alkali metals (Li, Na, K, …); *C.L Guillaume et al., Nat. Phys.,* ***7****, 211 (2011)*

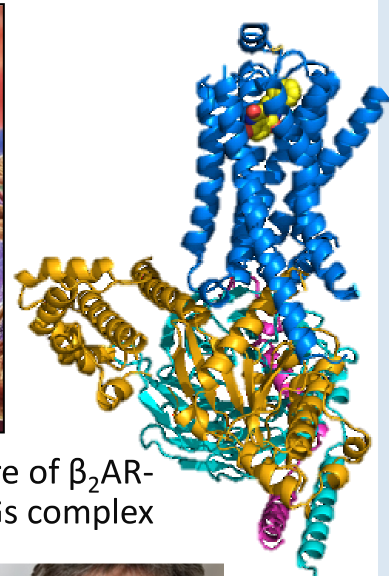
Life Sciences: Determining structure and dynamics from molecules to cells to organisms

Can we unravel the molecular mechanisms of living organisms?

Current Capability

APS leads world in protein crystallography



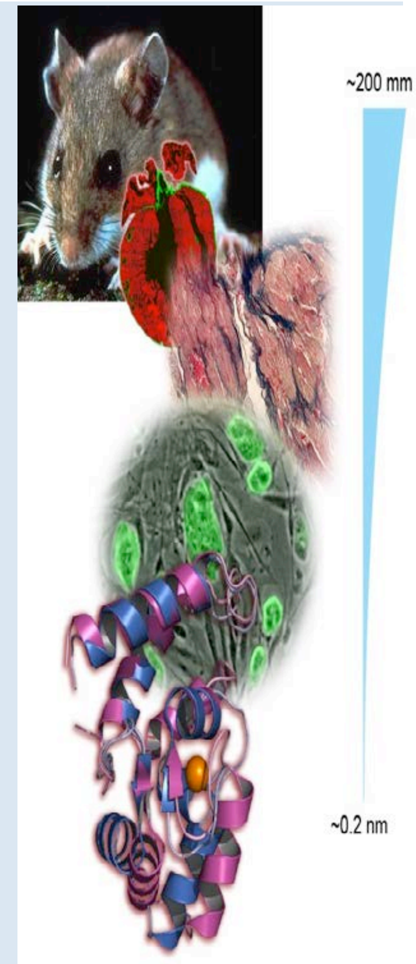


Structure of β_2AR-Gs complex

2012 Nobel Prize in Chemistry awarded to Kobilka and Lefkowitz for studies of G protein-coupled receptors

Capability leverages APS-U

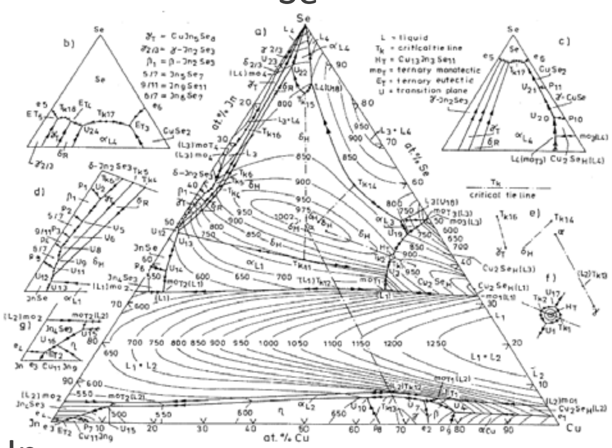
- 5x stability and high brightness needed for 1-µm MX; important for study of membrane proteins
- Imaging from 20 nm to 10 mm enables observation of structure/dynamics from genotype to phenotype
- High energies at APS reduce rad damage, provide access to all elements



DOW POWERHOUSE™ Solar Shingles: Reinventing the Roof

- In situ x-ray diffraction / differential scanning calorimetry studies by researchers from Dow Chemical using the DND-CAT beamlines at APS were used to investigate process / structure / property relationships in CuInGaSe materials (the active material in the first 'solar shingles').

Se



In

Cu

Research at APS (2007-2009)

Opening 2013

Will employ 1200 people by 2015

Phases, Kinetics, Processing → Manufacturing → Solar power that isn't on the roof, but IS the roof!

B. Landes, S. Rozeveld, B. Kern, B. Nichols, and J. Gerbi (Dow Chemical Co.)

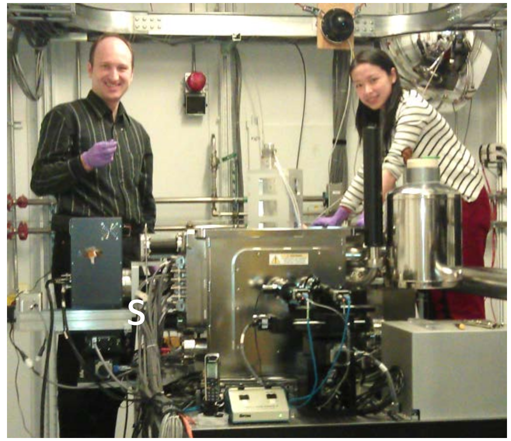
POWERHOUSE™ DOW SOLAR

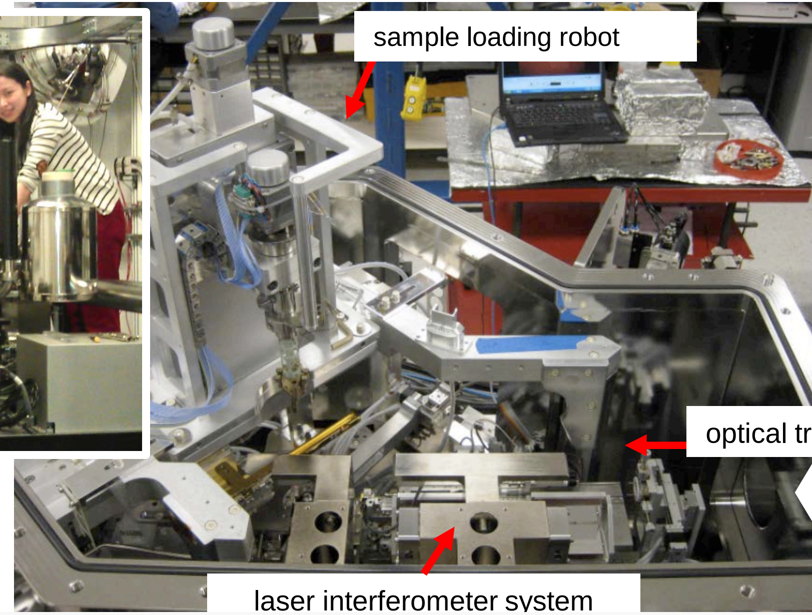
New Beamlines and Instruments Since Last 3-Way Meeting

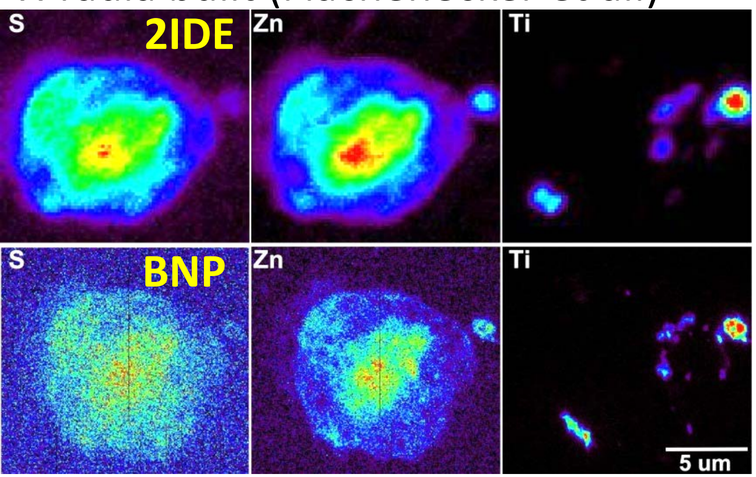
Beamline	Change	Research	First User Run
16-ID	cant	high pressure	2012-1
21-ID	new instrum.	bionanoprobe	2012-2
1-ID	new instrum.	diffraction microscopy	2012-2
13-ID	cant	geoscience	2012-3
7-BM	new beamline	µs radiography	2012-3
17-BM	conversion	powder diffraction	2012-3
1-BM	conversion	detectors, optics, topography	2013-1

21-ID Bionanoprobe

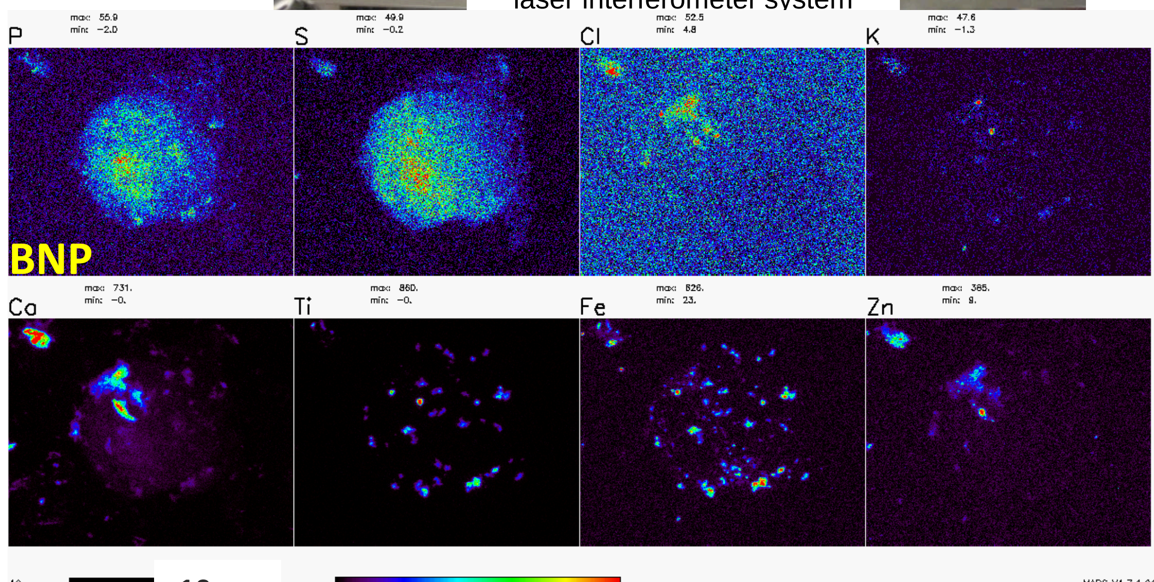
- Energy range: 5 – 20 keV
- resolution: 30 nm
- in vacuum **cryo**-system
- fast tomography
- instrument NIH/NCRR funded
- installed at LS-CAT
- collaboration Northwestern (Woloschak et al.), LS-CAT (Brister et al.), APS (Vogt et al.); X-radia built (Flachenecker et al.)







Comparison (at room temperature) of 'old' 2-ID-E microprobe (top), at 2s dwell time, with bionanoprobe (bottom) at 0.05 s dwell time, on a TiO2 nanoparticle exposed HeLa cell



Frozen-hydrated HeLa cells, treated with TiO2@Fe3O4-nanocomposites, imaged at cryogenic temperature with BNP, looking into how these nanoparticles move through cells

Argonne NATIONAL LABORATORY

NORTHWESTERN UNIVERSITY FEINBERG SCHOOL OF MEDICINE

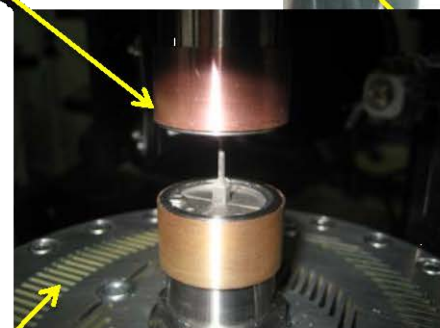
xradia insight in 3D

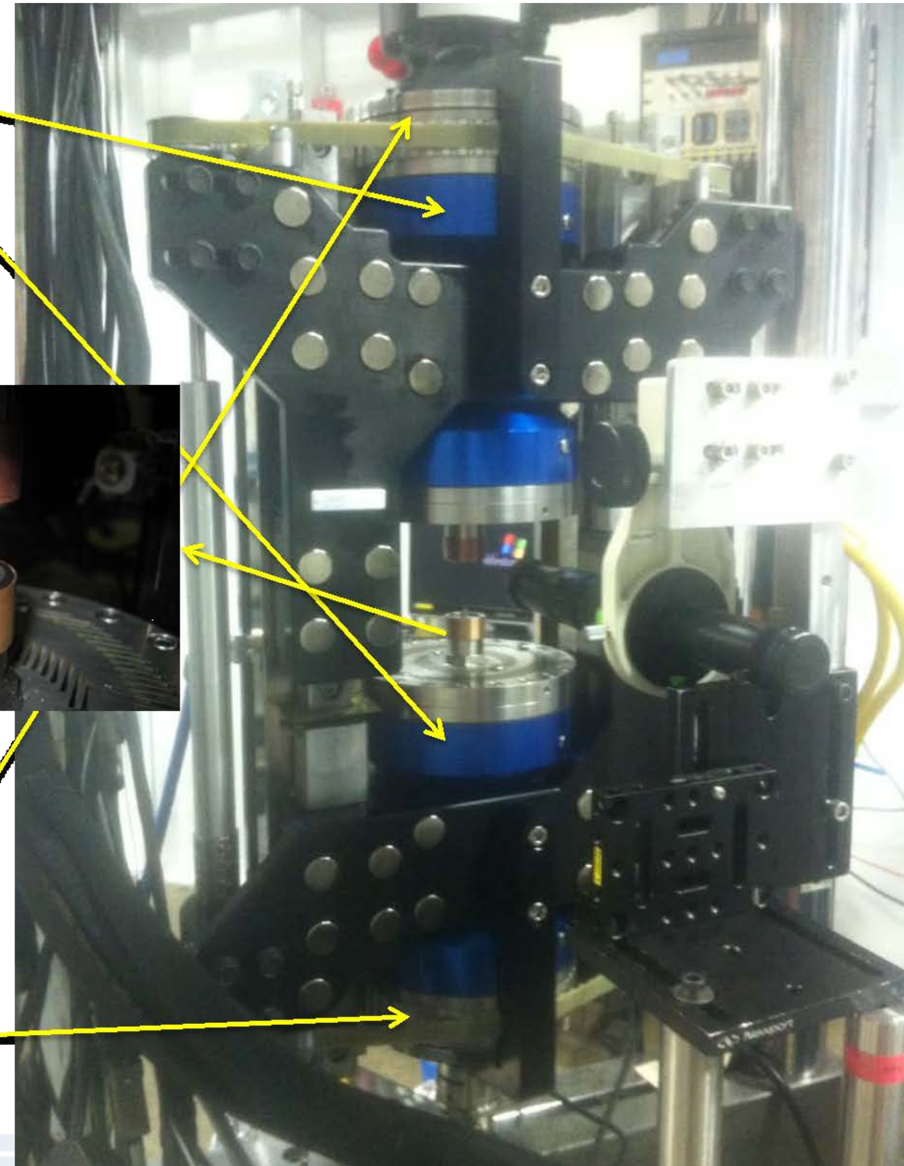
1-ID High-Energy In Situ Diffraction Tomography

- Partnership with Air Force Research Lab

Air bearing
sub assemblies for 360 degree
specimen rotation while under load

Thermally driven shrink fit grips to hold specimens while minimizing precession of the sample during rotation



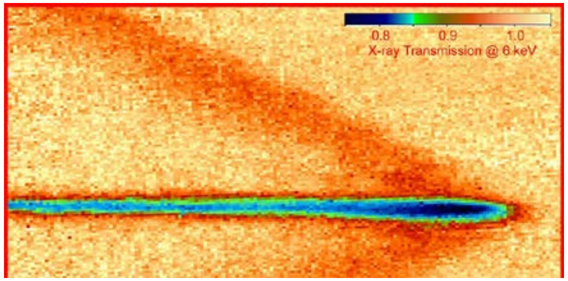


Flexure Plates for mechanical/rotation alignment where a 90 degree rotation of an allen wrench provides ~1 micron of specimen translation

Connected top/bottom drive system – control sample rotation to within 0.0015 degrees at up to 10 degrees/second

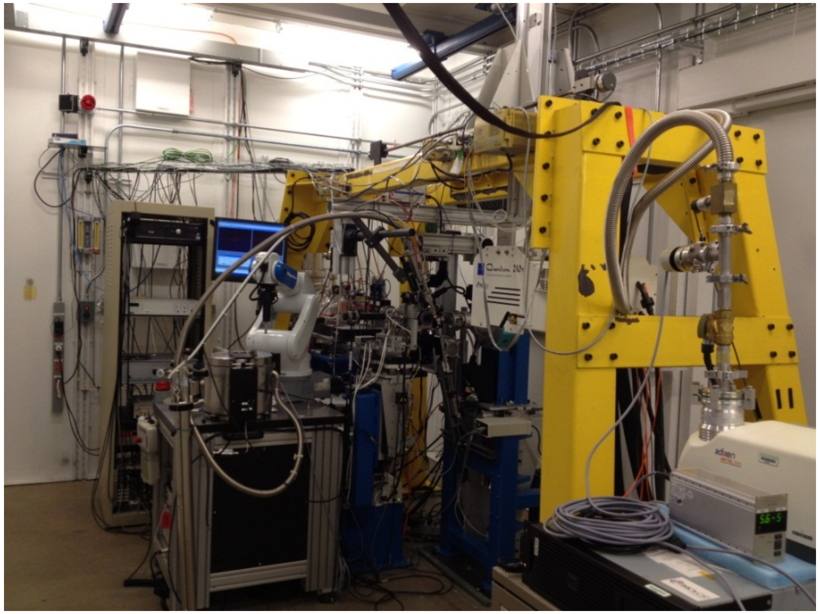
7-BM: DOE Vehicle Technologies

- Centralized facility for transportation engine technologies
  - high-throughput measurement
- OVT/EERE investment $850K capital
- μs x-radiography, μs x-tomography of fuel sprays, combustion
  - Wide-bandpass mono, >10^{13} ph/s full beam, 5.5 to 12 keV



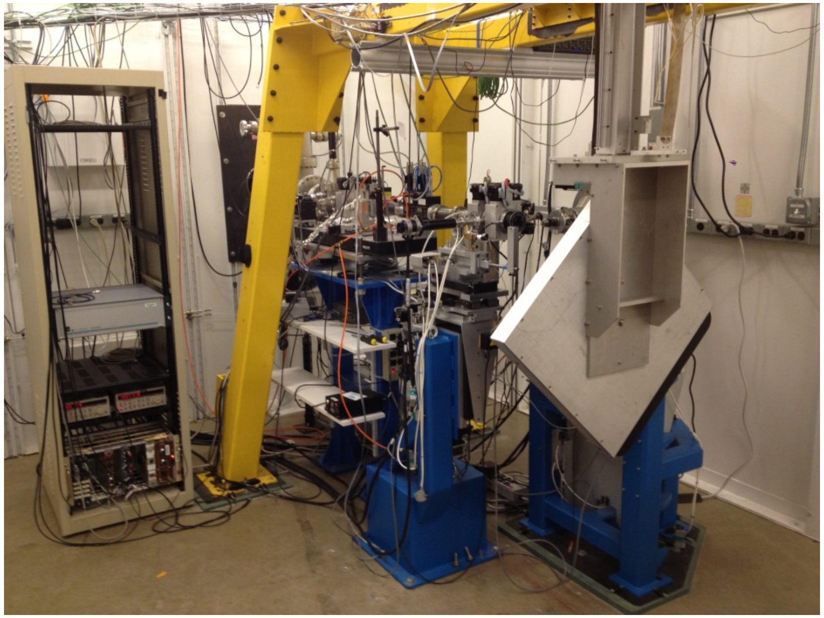
- Collaborators and partners from Argonne, industry, labs, and universities
  - Robert Bosch GmbH: diesel, and GDI
  - General Motor R&D: diesel
  - Visteon Corporation: GDI, HCCI
  - Delphi Corporation: diesel, GDI
  - Caterpillar: heavy duty diesel
  - Daimler AG: diesel, GDI
  - Continental AG (Siemens VDO): Diesel, GDI
  - Sandia National Lab
  - Air Force Research Lab
  - EPA
  - Argonne ES Division, Transportation Technology R&D Center
  - University of Wisconsin at Madison
  - Wayne State University
  - Cornell University
  - Michigan State University
  - Stony Brook University
  - Iowa University
  - University of Illinois at Chicago
  - University of California, Irvine

17-BM Powder Diffraction Conversion

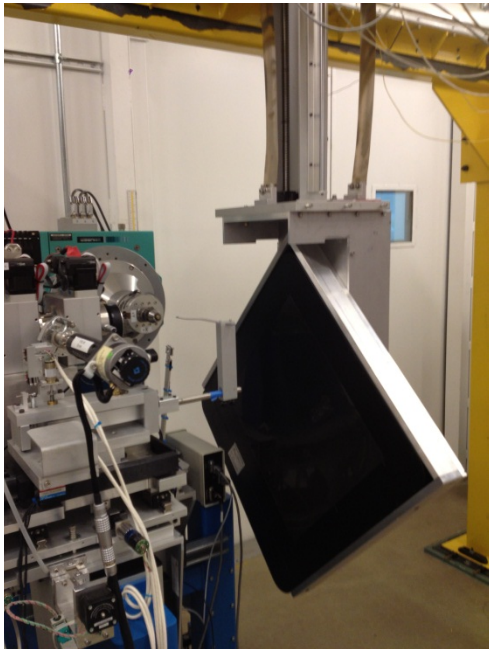


Original IMCA-CAT PX configuration

2012-3 first users:
in situ batteries,
high temperature,
high throughput,
high-pressure DAC

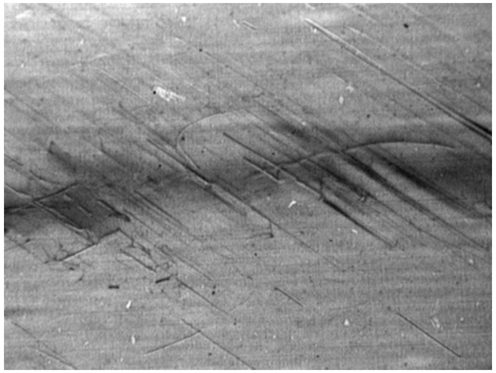


XSD powder diffraction configuration

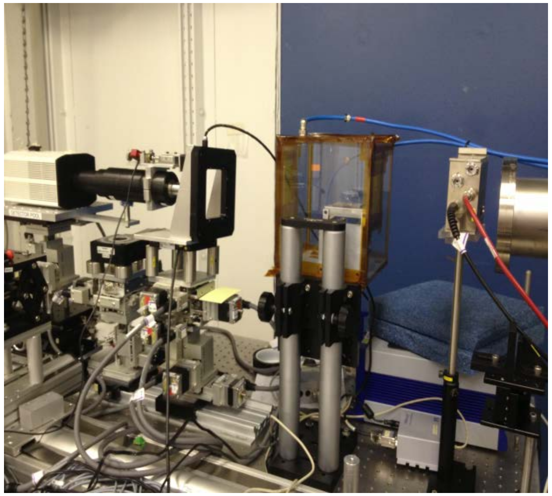


Reconfiguration of 1-BM

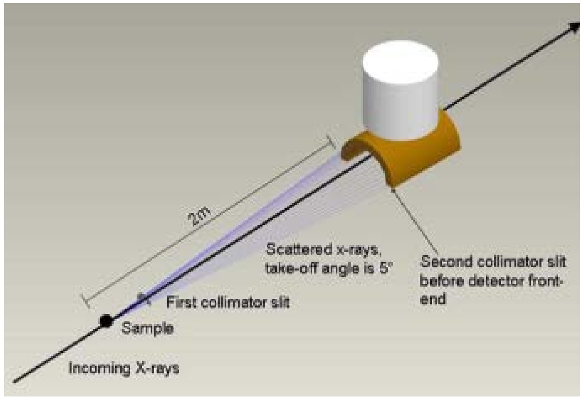
Optics Testing:
-- monochromatic beam topography available : 6- 30 keV
-- white beam topography coming in run 2013-1
-- Talbot interferometry available
Detector testing: available
Energy Dispersive Diffraction : planned for run 2013-1
High Energy Diffraction: planned
First external users Feb. 2013.



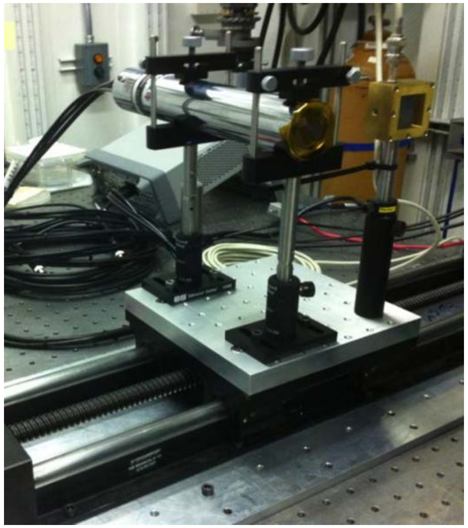
Topography example of materials screening for RIXS analyzers: unsuitable sapphire showing dislocations in 10 mm field of view taken at 1-BM



Interferometry set-up for K-B mirrors shown at 1-BM



Planned EDD arrangement

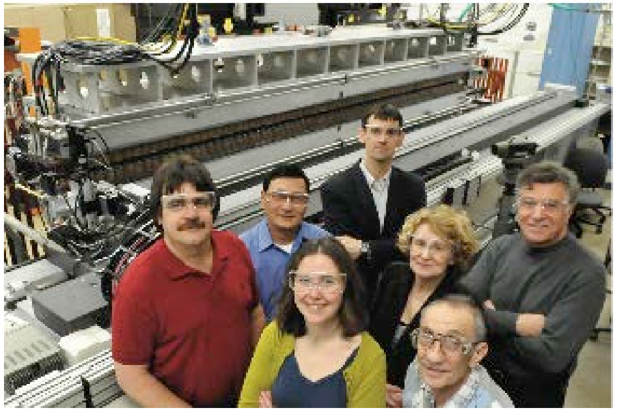


1-BM scintillation counter and p-i-n diode testing set-up at 1-BM

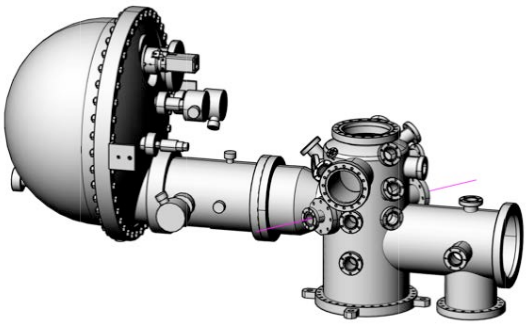
Intermediate Energy X-ray Sector 29 (Construction)

Collaborative development team with NSF and BES support led by J.C. Campuzano (UIC/ANL) and P. Abbamonte (UIUC/APS) to study collective excitations in interacting electron systems

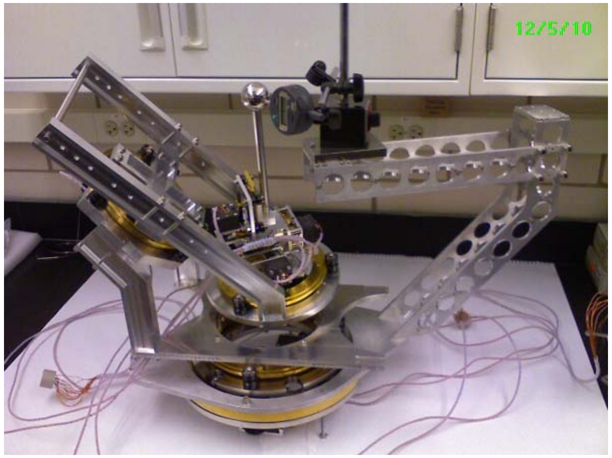
- Energy range: 250 eV – 3 keV
- Custom, quasiperiodic, electromagnetic EPU with variable polarization
- High-energy, angle-resolved photoemission (ARPES)
- Resonant scattering (RSXS) with energy analysis and κ geometry



IEX collaboration & electromagnetic EPU



Bulk-sensitive, high-energy ARPES system (under construction at UIC)

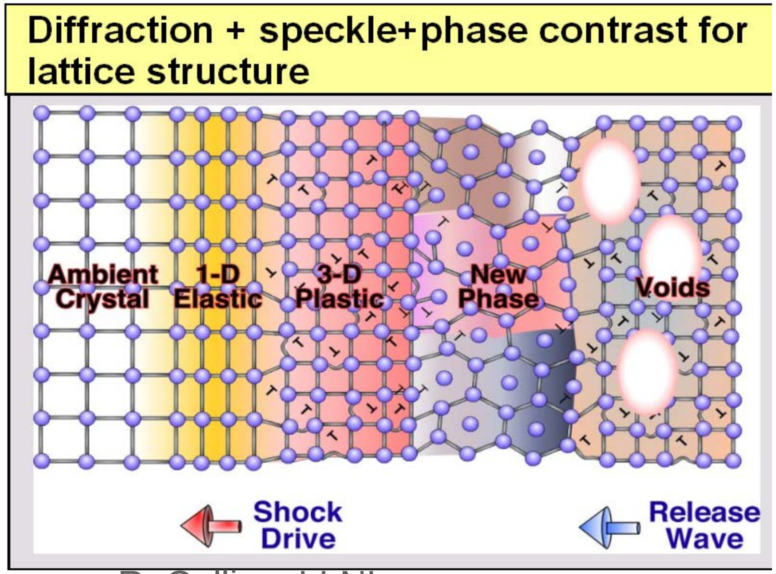


World's first soft x-ray diffractometer with κ geometry (built at UIUC)

Dynamic Compression Sector 35 (Construction)

Collaboration between Institute for Shock Physics (WSU), APS, NNSA, BES to study materials in real time under extreme conditions of pressure (e.g. shock waves)

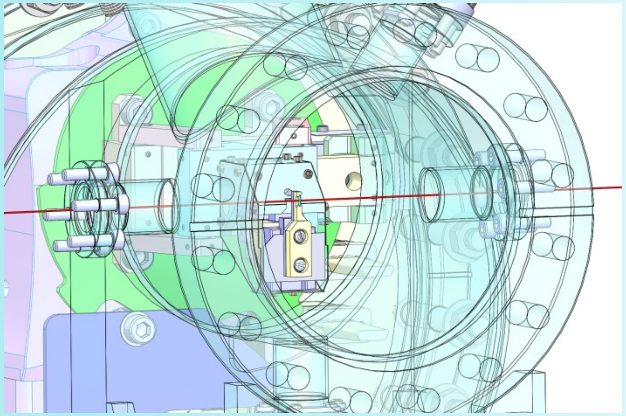
- Diffraction and imaging, 10 – 100 keV
- Time resolution down to 100 ps
- Dynamics of single events with ns to µs frame rates
- X-ray source, optics, hutches built by APS
- Drivers built and operated by WSU

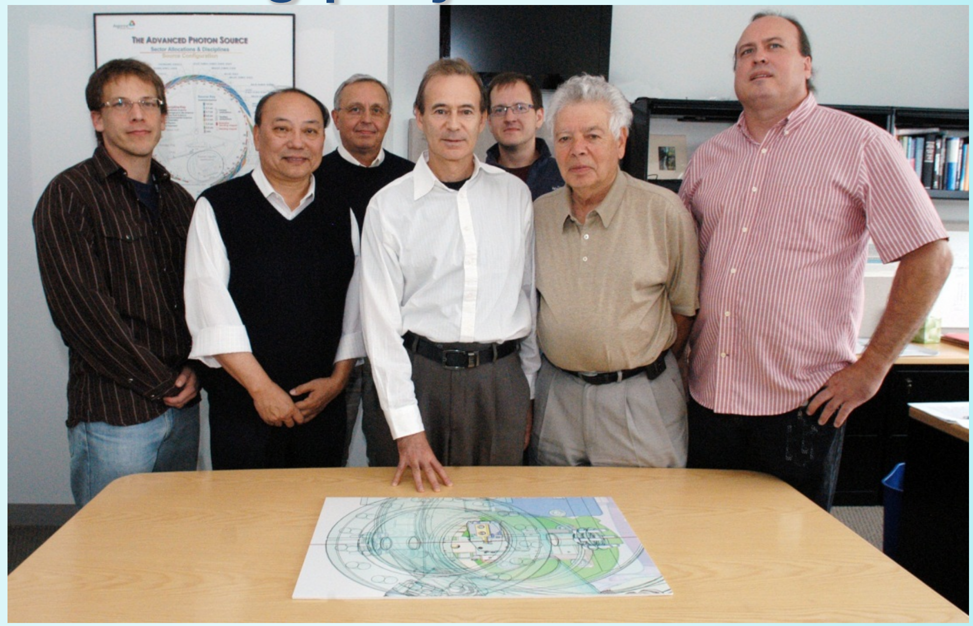


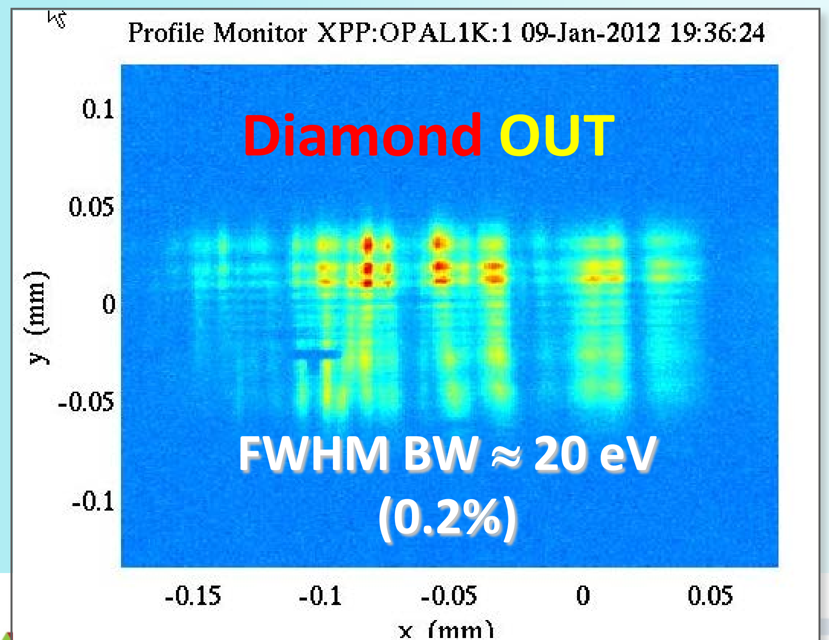
R. Collins, LLNL

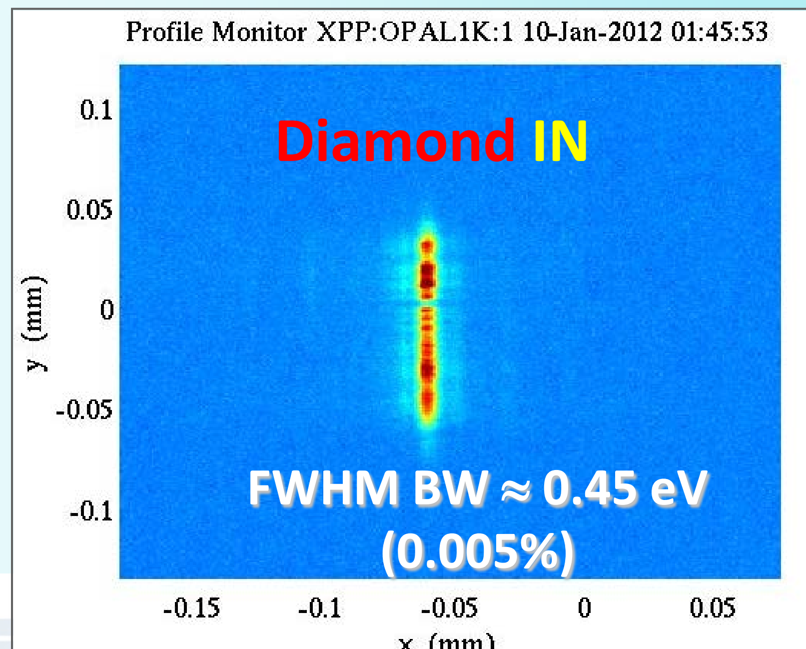
Hard x-ray self seeding project for LCLS

nature photonics





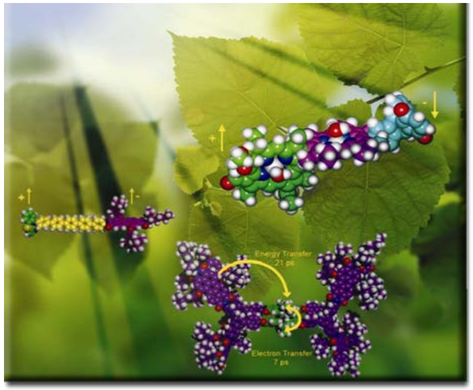




Advanced Protein Crystallization Facility Construction

- Funded by State of Illinois
- Space for ANL Biosciences programs
- Completion scheduled for Fall

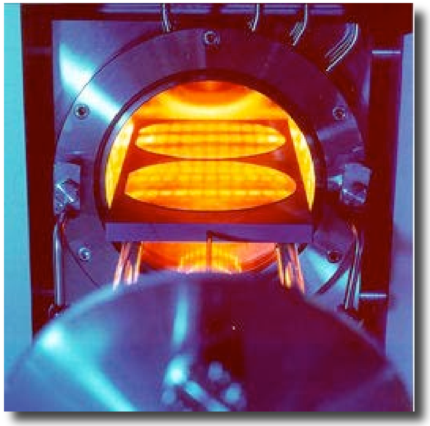
Two Scientific Themes Form the Basis for the APS Upgrade



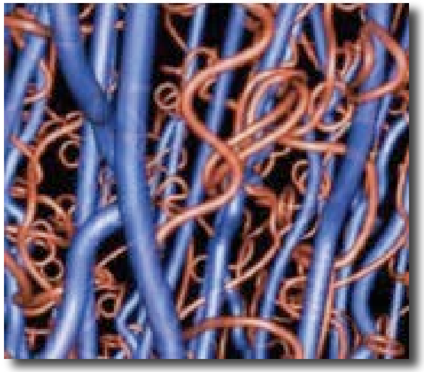
Can we harness photosynthesis for solar fuels?

Real materials under real conditions in real time

Mastering hierarchical structures through imaging

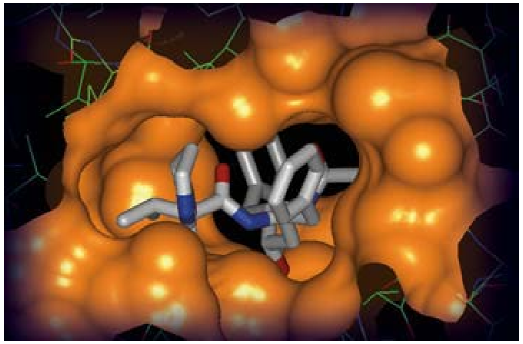


Can we control nucleation and growth to make better functional energy materials?



Is hydrogen an exotic metallic superfluid at 400 GPa?

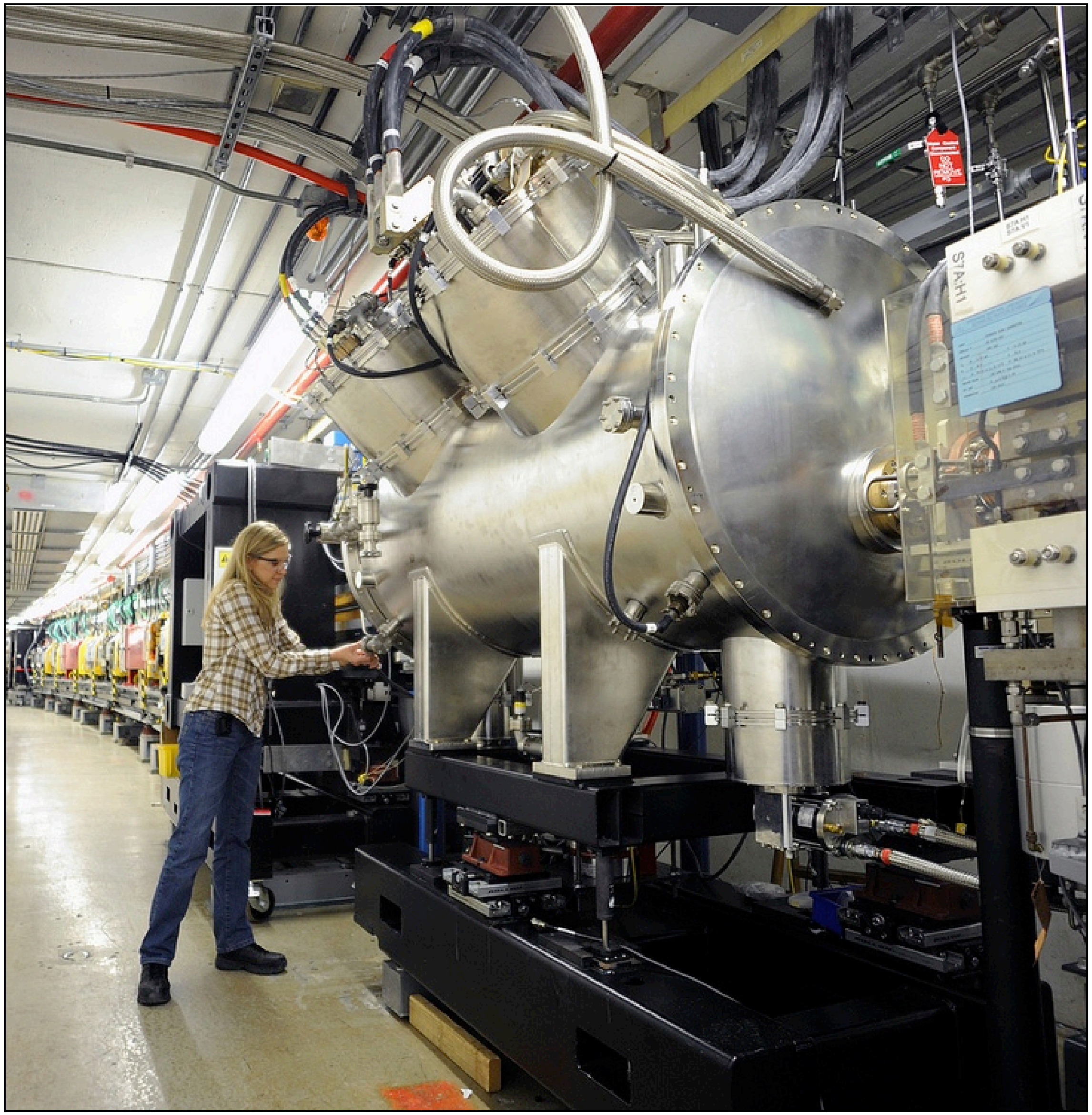
Addressing global issues in fundamental science, energy, the environment, and health



Can we design drugs that will effectively target disease?

Prototype Superconducting Undulator Operational

- 30-cm prototype SCU has been providing beam to users at Sector 6 ever since it was installed
- Exceeds design specs, very reliable, and already outperforms our standard undulator A at 85 keV
- 1-m SCU under construction



Prototype superconducting undulator installed in APS, December 2012

Thanks for your attention!