APS Update

G. Brian Stephenson

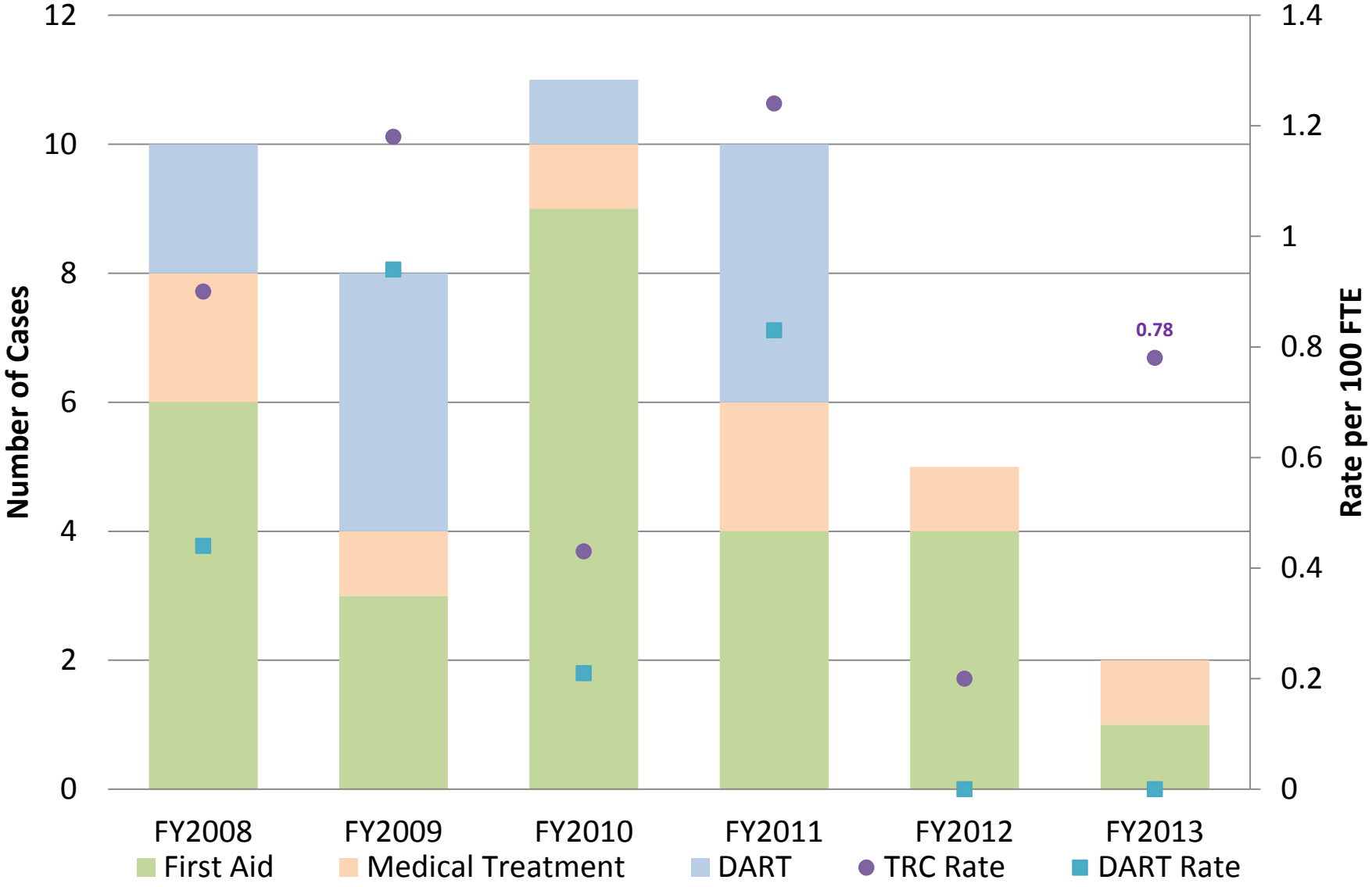
APSUOSC and APS PUC Joint Meeting

January 22, 2012

APS Update

- Safety
- Science Highlights
- New Beamlines and Instruments
- FY13 Projects
- FY13 Hiring, Space, Access Planning
- SAC Reviews of Beamlines
- DOE Budget Review
- Life Sciences Strategy
- Energy Storage Hub

APS Injury Types and TRC/DART Rate FY2008-13



eposits on the metal shell cable connector.

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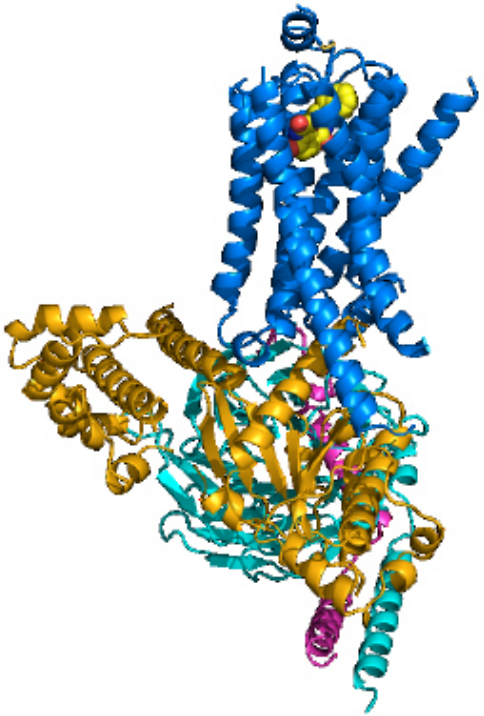
Work Planning & Control

- APS will be issuing a procedure for documenting work planning and control
- Three general categories of work are described:
  - Work performed using Skill of the Worker/Researcher
  - Work performed using step-by-step procedures
  - Specific work not covered by either of the above
- All experiments will continue to be documented by ESAF
- Hazard analyses and hazard controls for non-experimental work will be documented using a new Argonne web-based process
- CAT safety plans will need minor revision to address this new procedure
- A generic document for beamline operations hazard analysis and hazard controls will be prepared and will include most beamline non-experimental work
- Beamline staff may need to prepare some documents to address specific beamline unique hazards, especially if work procedures for these do not exist
- We will organize a meeting with beamline local managers and safety coordinators this Spring to discuss this in more detail

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"

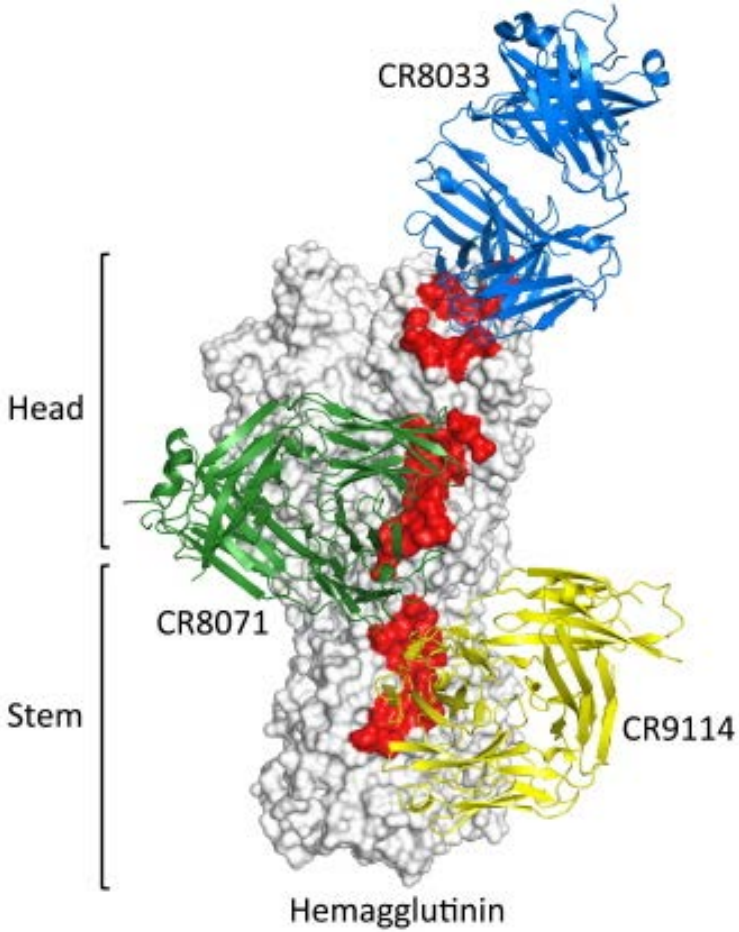
S.G.F. Rasmussen et al., Nature **477**, 549 (29 September 2011) DOI:10.1038/nature10361



The structure of the β_2AR-Gs complex

Outsmarting Flu Viruses

- Several biological protein structures were solved at GM/CA 23-ID, ALS, SSRL to study interaction of antibody CR9114 with group-2 influenza A viruses, allowing confirmation of broad neutralizing activity of antibody CR9114
- Paves way for development of universal vaccine for all influenza A and B viruses



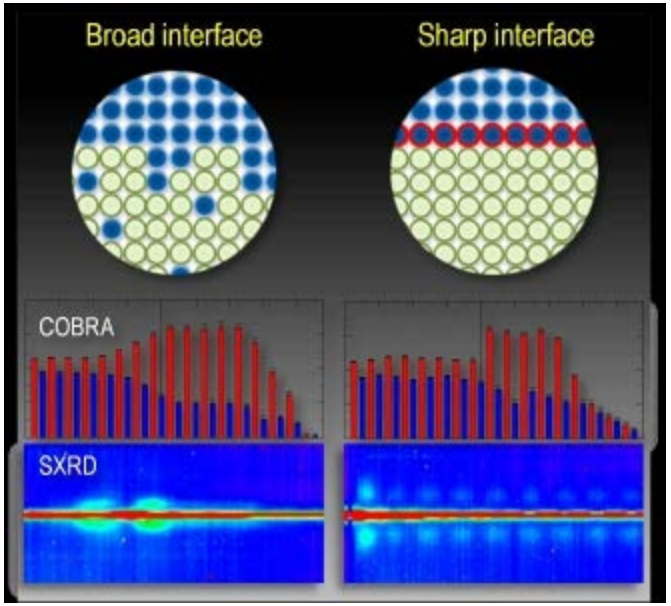
Surface representation of influenza hemagglutinin (white) with the newly identified sites of vulnerability colored red. Each site is unique and targeted by a different antibody. CR8033 (blue) binds to the head of HA, CR8071 (green) just below the head, while CR9114 (yellow) binds the stem. The stem binding CR9114, with its cross-neutralizing ability for influenza A and B viruses, provides proof of principle that a universal flu vaccine may be achievable.

C. Dreyfus, R. Khayat, D.C. Ekiert, J.H. Lee, Z. Metlagel, A.B. Ward, I.A. Wilson (The Scripps Research Inst.) N.S. Laursen (The Scripps Research Inst., Gustav Wieds Vej) T. Kwaks, D. Zuijdgeest, M.V. Bujny, M. Jongeneelen, R. van der Vlugt, M. Lamrani, H.J.W.M. Korse, E. Geelen, Ö. Sahin, M. Sieuwerts, J.P.J. Brakenhoff, R. Vogels, W. Koudstaal, J. Goudsmit, R.H.E. Friesen, (Crucell Vaccine Inst.) O.T.W. Li, L.L..M. Poon, M. Peiris (The U. of Hong Kong)

C. Dreyfus.et al., "Highly Conserved Protective Epitopes on Influenza B Viruses," Science **337**, 1343 (14 September 2012).

Engineering Thin-Film Oxide Interfaces

- High-energy x-rays at XSD 12-ID and 33-ID reveal electrical conductivity at interface between two oxide insulators
- Helps resolve mysterious origin of conductivity in epitaxially-grown lanthanum aluminate ($LaAlO_3$) and strontium titanate ($SrTiO_3$) thin films
- New insights about material that might form basis for alternative to conventional silicon-based semiconductor technology
- Explored effects of high and low oxygen pressures on physical properties of thin-film LAO/STO systems produced using pulsed laser deposition
- Highly sensitive diffraction enabled by extreme brightness x-rays allowed study of the structure, composition of LAO/STO near-interface region with unprecedented detail



Electron densities obtained by COBRA and real-time surface x-ray diffraction during film growth show that a chemically abrupt interface can be produced by inserting a monolayer-thick buffer grown in high pressure with the rest of the thin-film structure grown at low pressure.

W.S. Choi, C.M. Rouleau, G.Eres, M.F. Chisholm, H.N. Lee (ORNL) S. S.A. Seo (ORNL & U. Kentucky) Z. Luo (ANL, U. Science and Technology of China) H. Zhou, T.T. Fister, J.A. Eastman, P. H. Fuoss, D.D. Fong, J.Z. Tischler, (ANL)

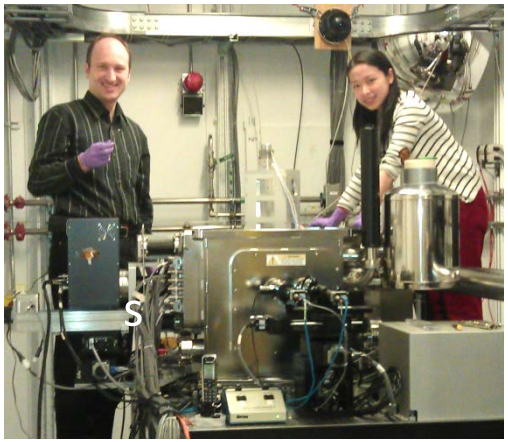
W. S. Choi et al., "Atomic Layer Engineering of Perovskite Oxides for Chemically Sharper Heterointerfaces," Adv. Mater., published online 4 October, 2012.

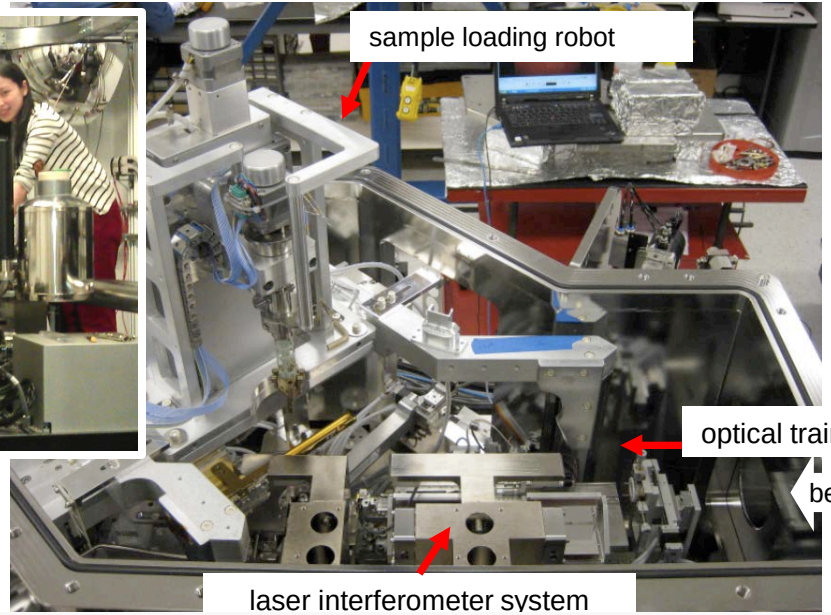
New Beamlines and Instruments

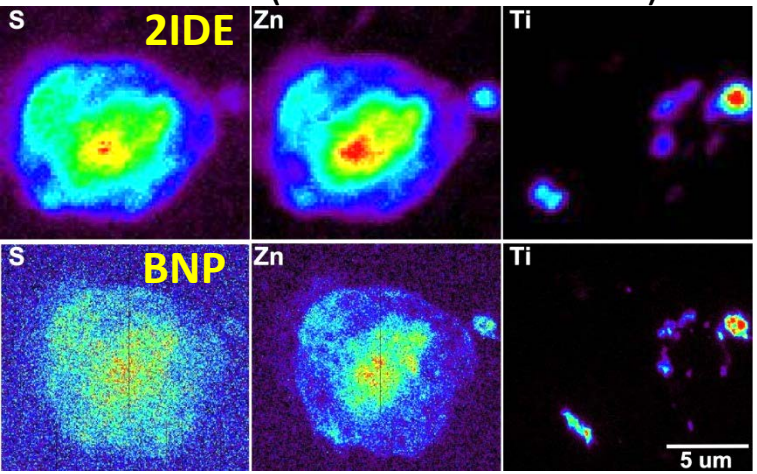
Beamline	Change	Research	First User Run
34-ID	cant	imaging	2011-3
16-ID	cant	high pressure	2012-1
21-ID	new instrum.	bionanoprobe	2012-2
1-ID	new instrum.	diffraction tomography	2012-2
13-ID	cant	geoscience	2012-3
7-BM	new beamline	µs radiography	2012-3
17-BM	conversion	powder diffraction	2012-3
1-BM	conversion	detectors, optics, tompography	2013-1

21-ID Bionanoprobe

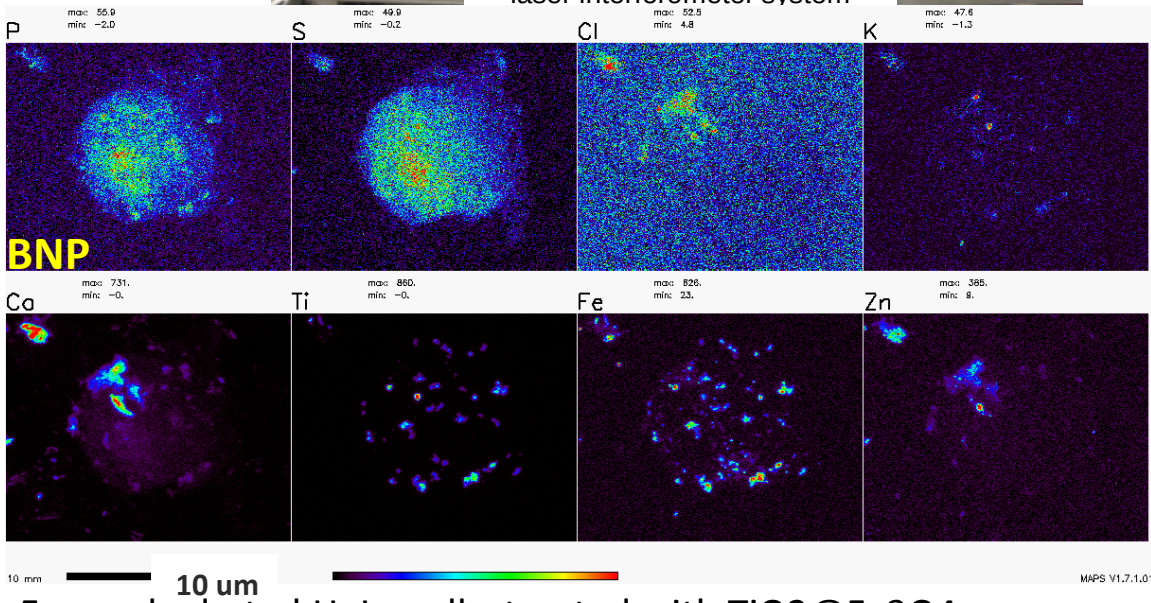
- Energy range: 5 – 20 keV
- resolution: 30 nm
- in vacuum **cryo**-system
- fast tomography
- instrument NIH/NCRR funded
- installed at LS-CAT
- collaboration Northwestern (Woloschak et al.), LS-CAT (Brister et al.), APS (Vogt et al.); X-radia built (Flachenecker et al.)







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

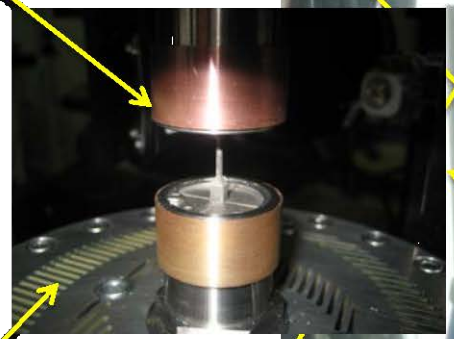
xradia insight in 3D

1-ID High-Energy In Situ Diffraction Tomography

- PUP with Air Force Research Lab

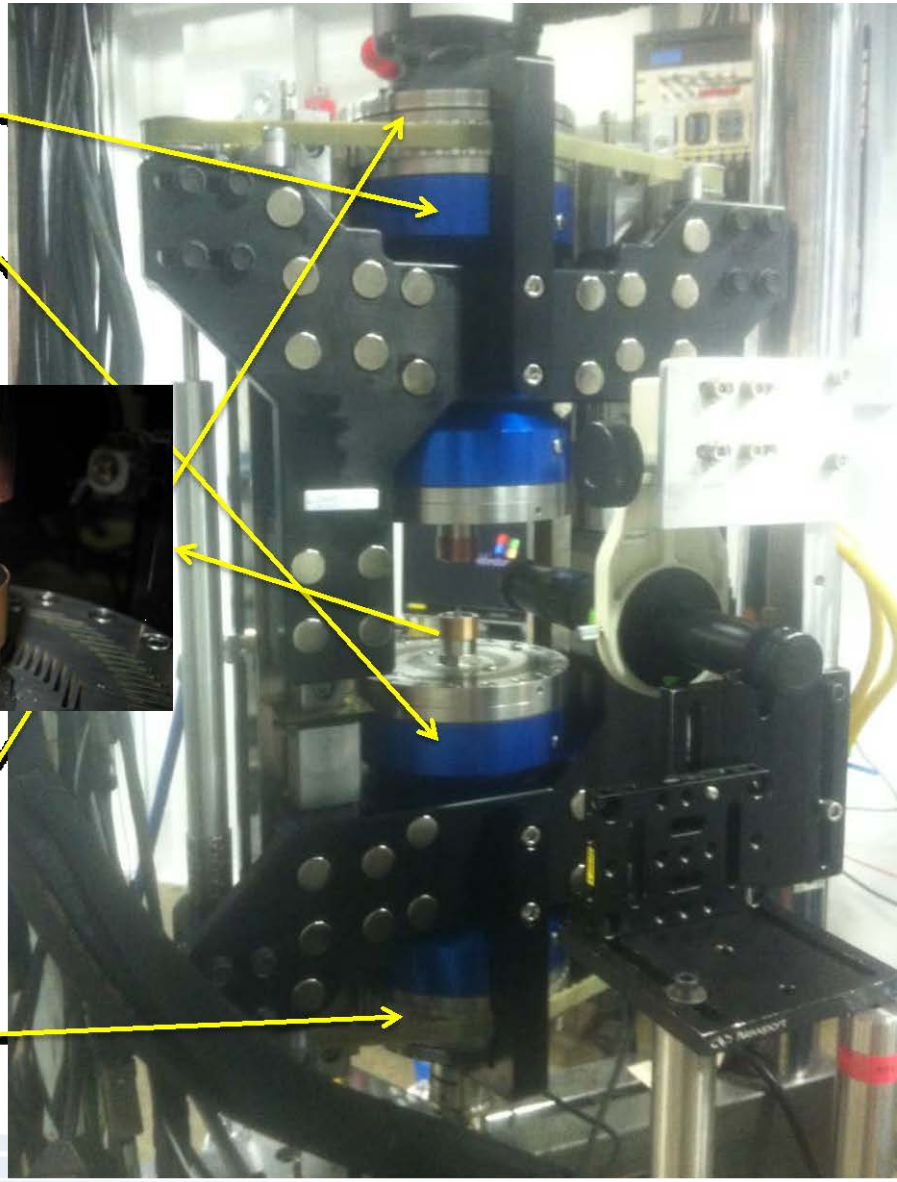
Air bearing
sub assemblies for 360 degree specimen rotation while under load

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

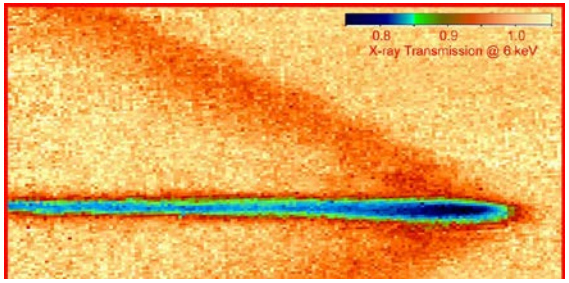


Flexure Plates for mechanical/rotation alignment where a 90 degree rotation of an allen wrench provides ~1 micron of specimen translation

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

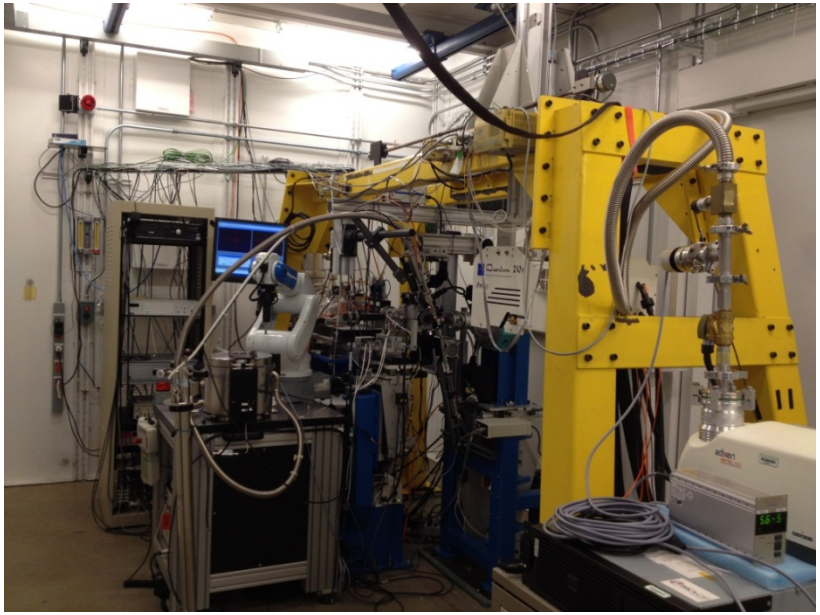


7-BM: DOE Vehicle Technologies

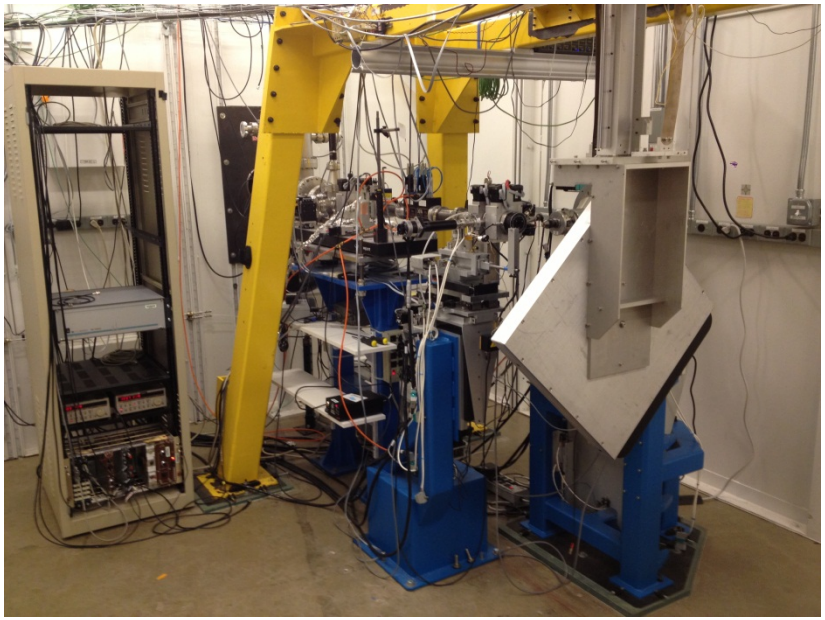


- Centralized facility for transportation engine technologies
  - high-throughput measurement
- OVT/EERE investment $850K capital
- µs x-radiography, µs x-tomography of fuel sprays, combustion
  - Wide-bandpass mono, >10^{13} ph/s full beam, 5.5 to 12 keV
- Collaborators and partners from Argonne, industry,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

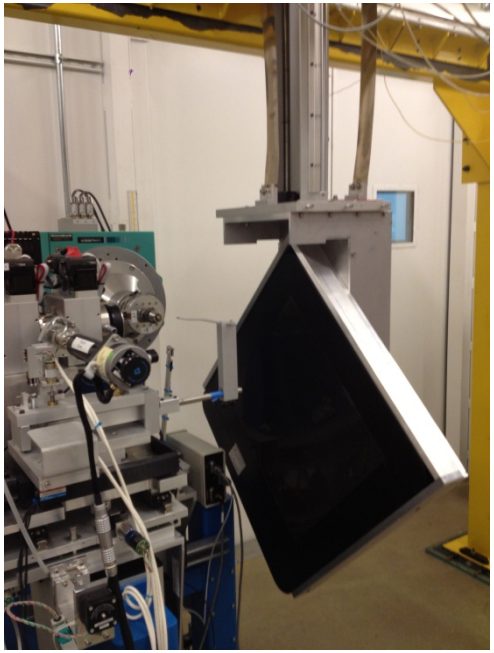
17-BM Powder Diffraction Conversion



Original IMCA-CAT PX configuration



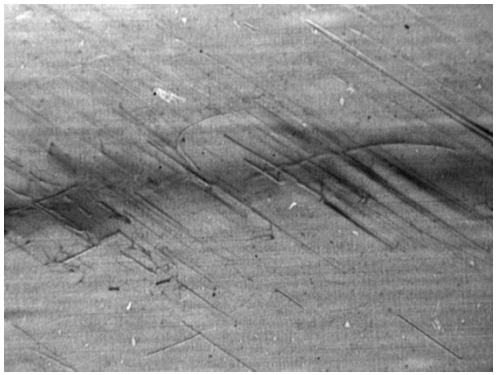
XSD powder diffraction configuration



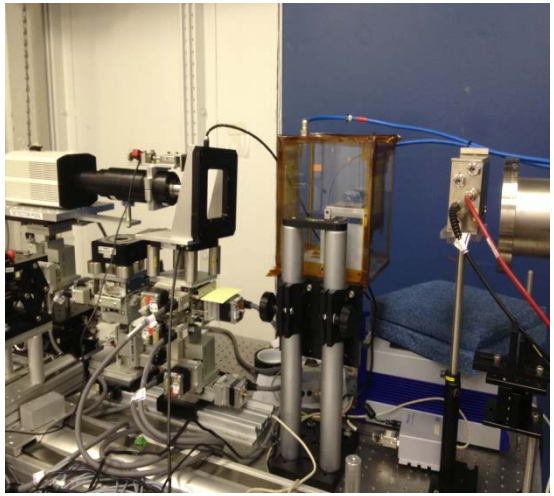
2012-3 users scheduled:
in situ batteries,
high temperature,
high throughput,
high-pressure DAC

Reconfiguration of 1-BM

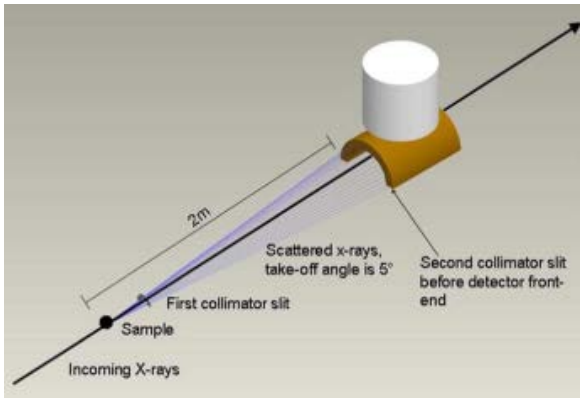
Optics Testing:
-- monochromatic beam topography available : 6- 30 keV
-- white beam topography coming in run 2013-1
-- Talbot interferometry available
Detector testing: available
Energy Dispersive Diffraction : planned for run 2013-1
High Energy Diffraction: planned
First external users scheduled for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



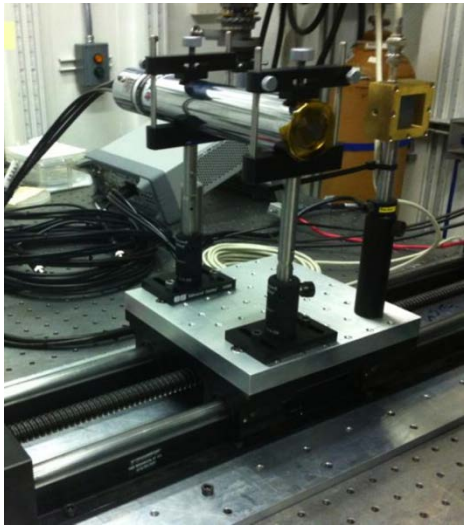
Topography example of materials screening for RIXS analyzers: unsuitable sapphire showing dislocations in 10 mm field of view taken at 1-BM



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

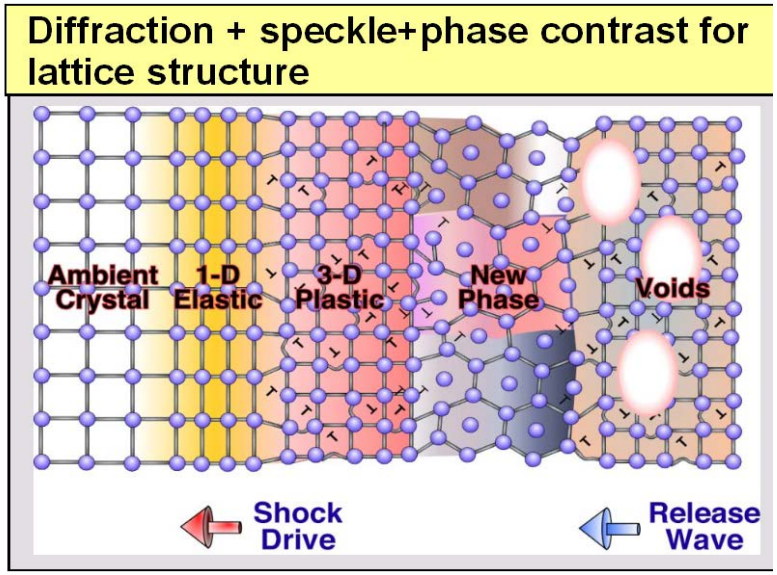
FY13 Plans

- New / Expanded Beamlines
  - 29-ID Intermediate Energy X-ray (IEX)
  - 1-BM Detectors/Optics/Topography
  - 14-ID Ultrafast Scattering for Physical Sciences
  - 35-ID DCS Construction
- Equipment Projects
  - Cryostat for 2nd superconducting undulator to allow SCU0 to remain in operation at 6-ID
  - Computer server upgrades
  - High-energy diffraction instrumentation

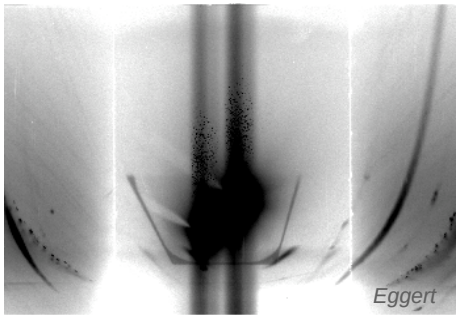
Real-Time, Microscopic Measurements at Extreme Conditions

- Integrates NNSA and SC expertise to understand materials behavior under extreme conditions of dynamic compression at microscopic length scales and nanosecond time scales
- First-of-a-kind dedicated capability: in situ time-resolved diffraction and imaging during dynamic compression
- Global DCS user base (16 national and international institutions)
  - NNSA, DoD labs, universities
  - International institutions (UK, India, Japan, S. Korea, and Germany)

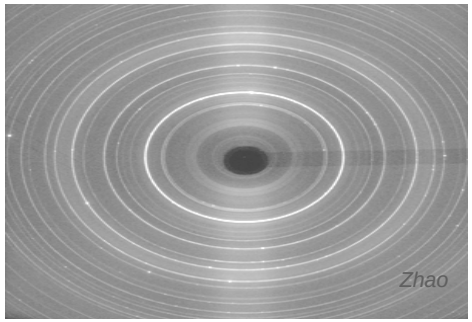
- WSU/APS partnership to develop and operate DCS at Sector 35



R. Collins, LLNL



Current Dynamic Diffraction

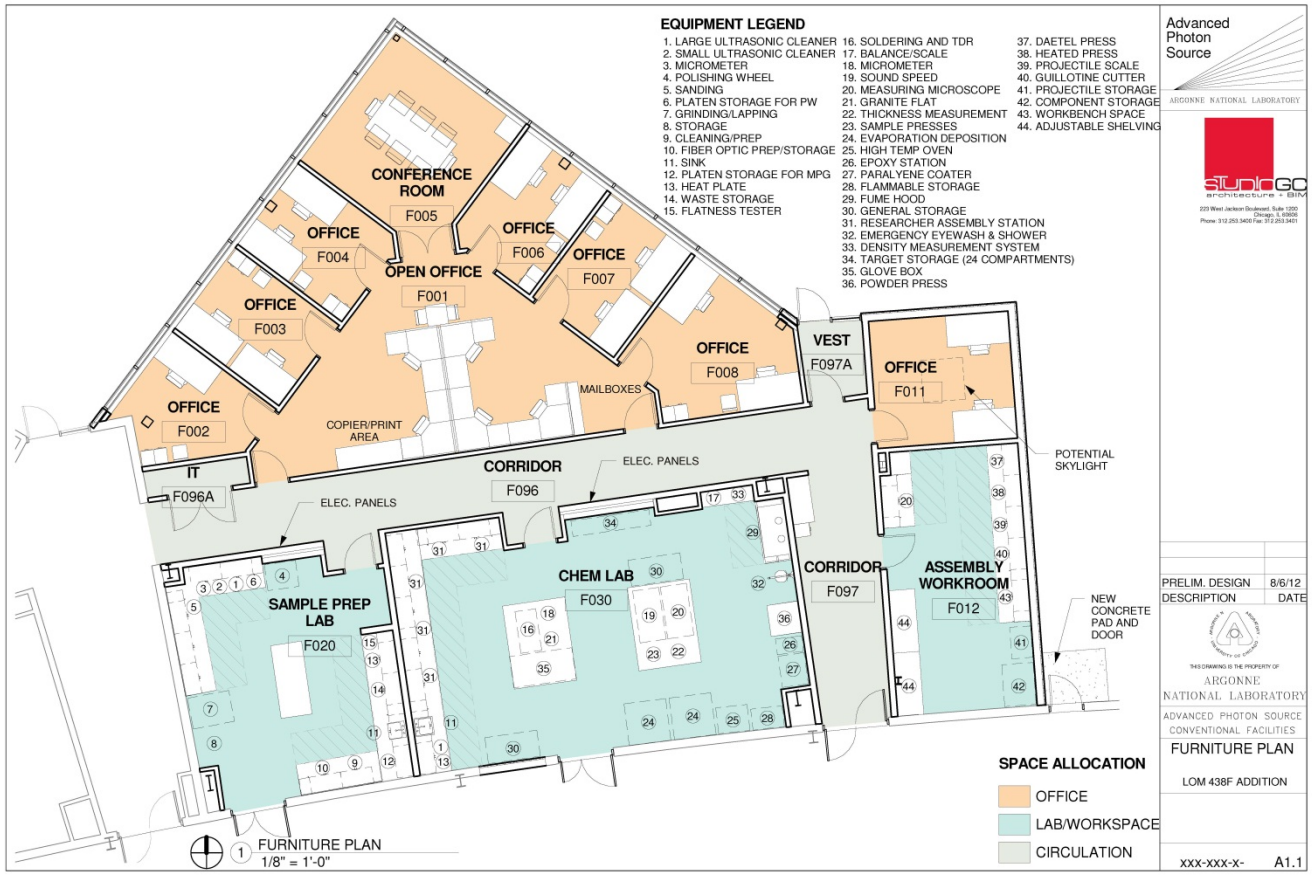


APS Dynamic Diffraction

DCS Project LOM 438F Pentagon

LOM 438F
Under Constr.

DCS Project LOM 438F Pentagon

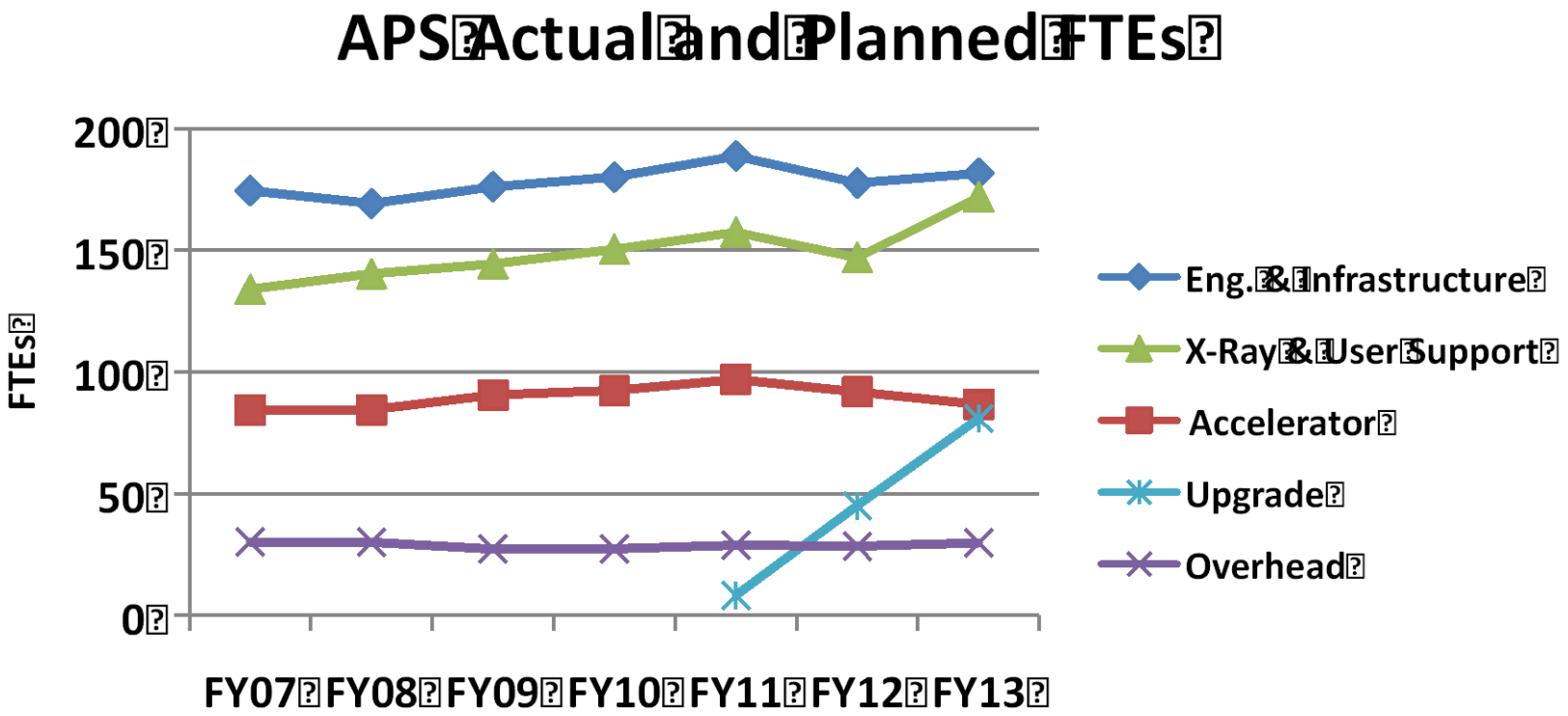


Dynamic Compression Sector (DCS) Project

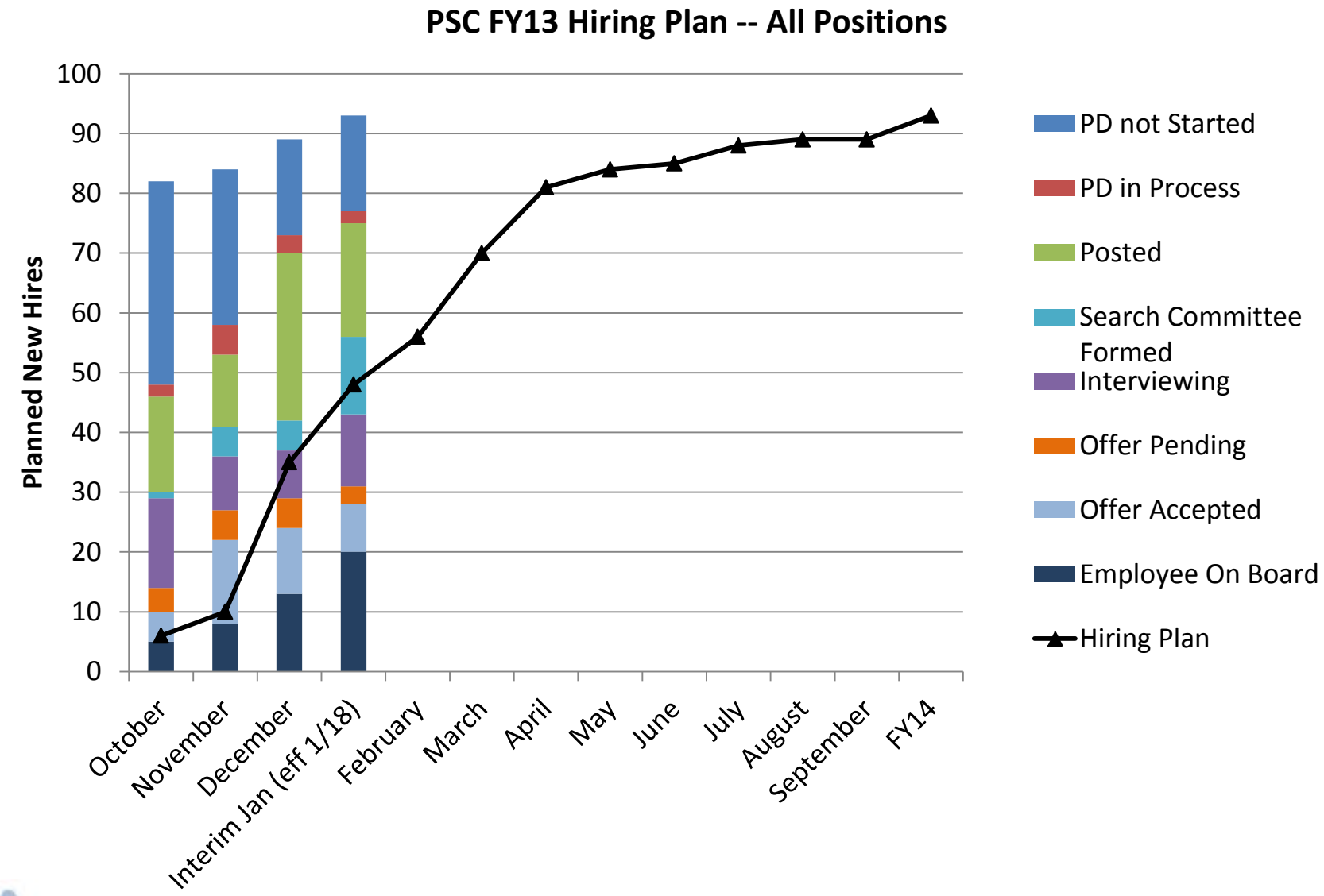
Sector 35 Upstream Area

APS Staffing Increases, Driven by the Upgrade

- FY12:
  - 46 staff hires
  - 6 postdoc hires
  - 14 contractors
  - (22 terminations)
- Plan for FY13:
  - 80 staff hires
  - 10 postdoc hires



APS Hiring Progress in FY2013



Office Space in FY2013

- The plan calls for 90 new hires for FY2013 – where will we put them?
  - Selected areas of Building 401 are being reworked to make room for more people.
  - More people (and equipment) will be moved into Building 314.
  - Buildout of the offices in LOM 437 is planned for FY2013. When complete, LOM 437 will be able to house at least 40 people.
  - The Guest House will be used for temporary accommodation. It is economical and office spaces are available. APS has ~15 people there now. The Guest House can absorb another 60 people in office spaces if required, and can be used for temporary accommodation e.g. until LOM 437 is complete.

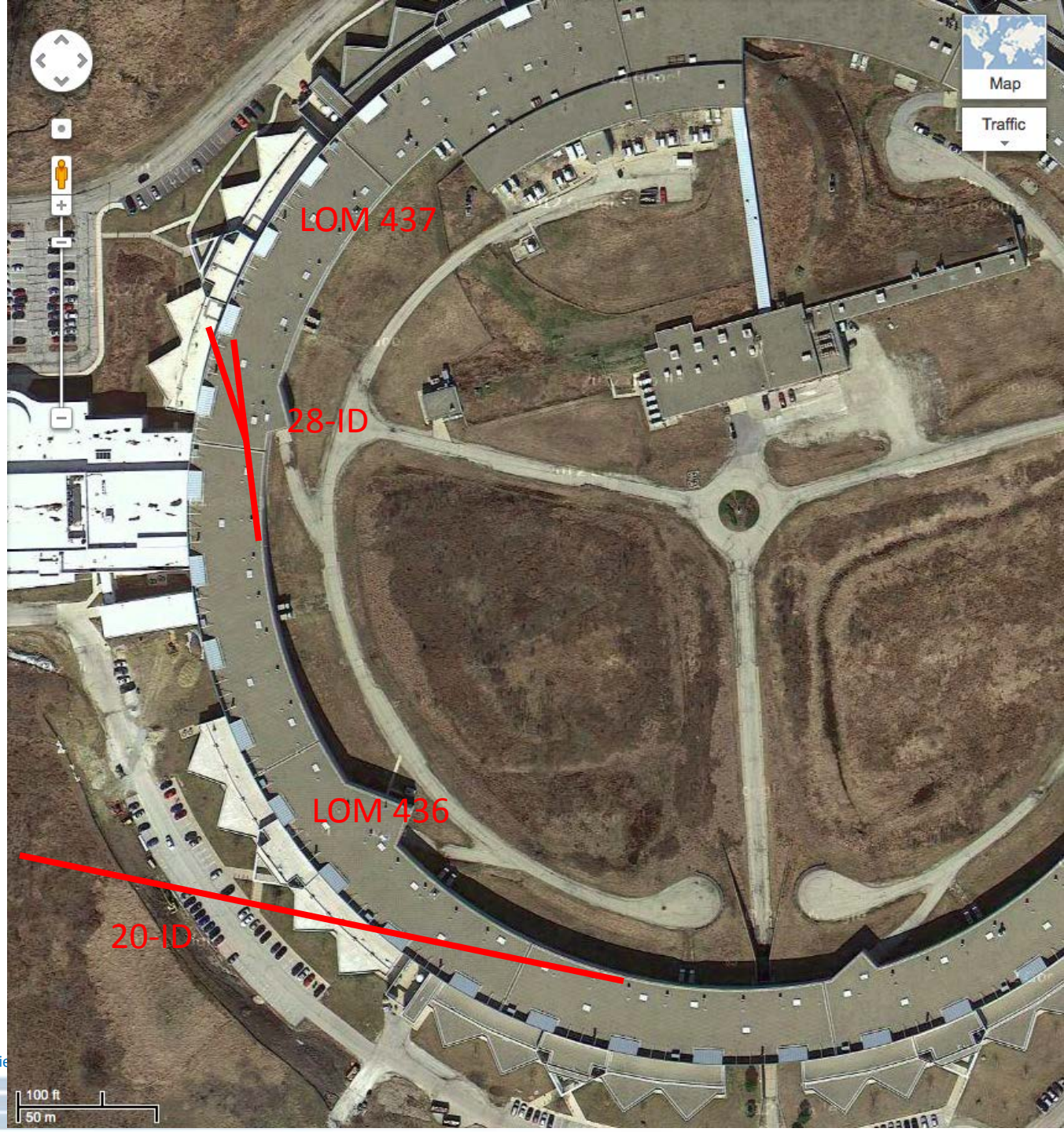
LOM 437 Contents Being Moved

New MOM Technician Area

This space was the Exercise Room adjacent to the Lower Gallery
Provides office space for techs previously in Sector 35 area

Access Planning

- Future beamlines will block the main aisle at 20-ID and 28-ID
- Will need external truck access between
- Foot traffic via stairway over 20-ID at aisle and walkway around 28-ID through LOM 437
- Should we continue to use tricycles?
- New building next to CNM and potential rebuild of LOM 436 are being considered



APCF Construction Progressing

- Foundation and steel structure is complete
- "Topping out" celebration 1/14/2013

SAC Beamline Reviews: October 3, 2012
Panel A: HERIX and NRS

- Beamlines reviewed: 3-ID and 30-ID (HERIX)

- Review Panel:

  Dan Neuman (SAC, NIST), Chair

  Mark Sutton (SAC, McGill)

  Chi-chang Kao (SSRL)

  Jay Bass (UIUC)

  Steve Durbin (Purdue)

  Laura Greene (UIUC)

SAC Beamline Reviews: October 3, 2012
Panel B: SAXS, WAXS, GISAXS, USAXS, and XPCS

- Beamlines reviewed: 8-ID-E, 8-ID-I, 12-ID-B, 12-ID-C/D, (SAXS/WAXS only), 15-ID (USAXS only)

- Review Panel:

  KaYee Lee (SAC, UofC), Chair

  Friso van der Veen (SAC, Paul Scherrer)

  Roger Leach (SAC, DuPont)

  Jack Johnson (SAC, Scripps)

  Soichi Wakatsuki (SAC, Photon Factory)

  Andrei Fluerasu (BNL)

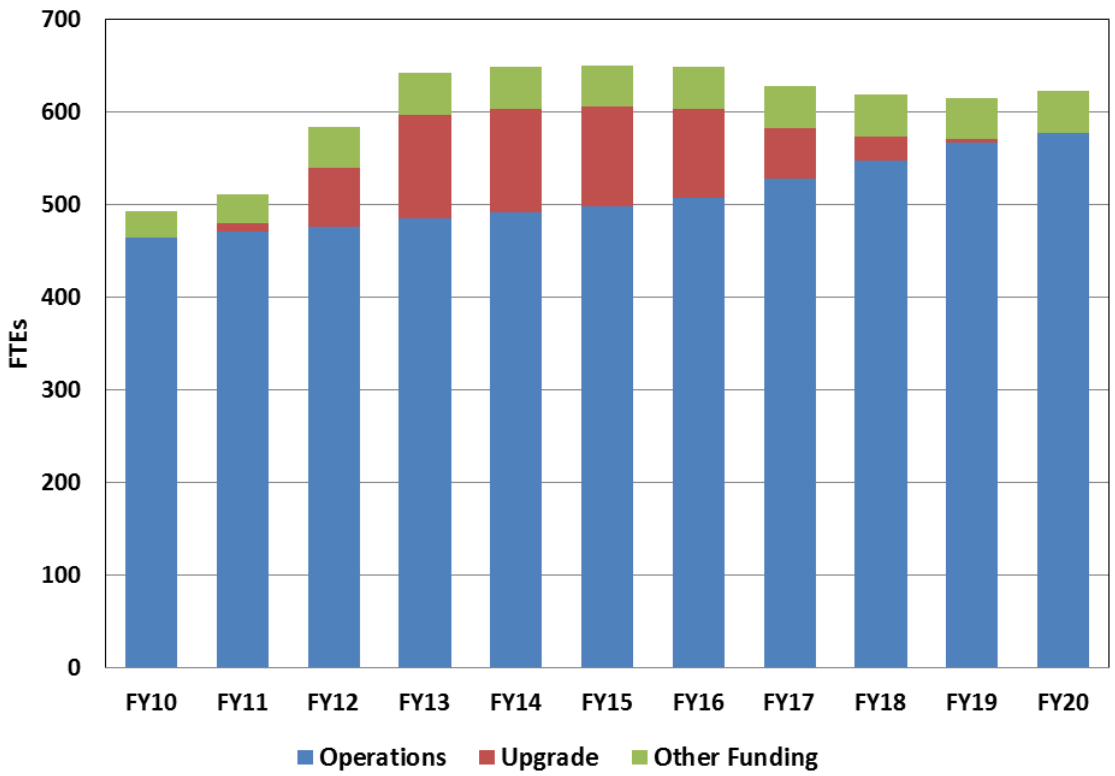
Upcoming SAC Beamline Reviews: March 5, 2013

- Panel 1: Industrial MX: 17-ID (IMCA) and 31-ID (LRL)
  - SAC chair: Jack Johnson
- Panel 2: 10-ID, 10-BM (MR)
  - SAC chair: Mark Sutton
- Panel 3: 16-ID, 16-BM (HP)
  - SAC chair: Glenn Waychunas

Upcoming BES Review of Facilities Operations Budgets

- After a review of the NSLS-II proposed budget last fall, DOE BES will be reviewing the operations budgets of their other light sources (ALS, SSRL, LCLS, APS) this Spring

- The APS review is scheduled for May 16-17
- We will present our plans for the next decade



Potential Joint Approaches by Life Sciences Community with APS to Federal Agencies

Since the founding of the APS, structural biology CATs have sought funding independently of one another for their initial construction, operations and upgrades. CATs have been very successful in obtaining funding from a wide variety of sources, and now operate under a range of models

Are there projects for which CATs might now seek joint funding?
Life Sciences Council : YES

Three candidate areas for such projects identified:

- activities related to the NSLS dark period e.g. funding for staff added to accommodate increased demand at APS, or to increase efficiency and capacity of remote access by users (short to medium term; limited time frame; likely to affect many CATs; relatively low cost)
- hardware upgrades to structural biology beamlines to take full advantage of APS Upgrade (medium term; limited time frame; likely to affect most, perhaps all CATs; medium cost)
- construction and operation of new beamlines e.g. those that form part of the DOE-OBER Proteins to Organisms plan, further reviewed by the SAC in March 2011 as part of the APS-U overview (medium to long term; likely to broaden scope of some CATs and affect others; high cost)

APS MX Resources for NSLS-I to NSLS-II Transition

Potential Beamline Resources Available
for
Life Sciences
at the
Advanced Photon Source
Argonne National Laboratory

Slides sent to Amy Swain (NIH) and Roland Hirsch (BER)
November 2012

NSLS MX User Access to APS Beamlines

- MX beamlines at APS are operated by CATs
  - CATs provide a minimum of 25% of beamtime to General Users
  - Several CATs operate as National User Facilities and give a much larger percentage to General Users, up to 100%
- NSLS users can apply for beamtime on any APS beamline as General Users
  - Proposals are scored by external reviewers
  - Based on score and requirements, beamtime may be allocated on ID or BM beamlines
- To make sufficient MX beamtime available for displaced NSLS users as well as the current APS user community, we propose to increase capacity through
  - access to underutilized bending magnet beamlines
  - improved efficiency at some ID beamlines
- The following table indicates the approximate increase in capacity that can be obtained and the resources (equipment and staffing) needed
  - NSLS staff could temporarily relocate to Chicago and help provide user support
  - If funds are available new staff could be hired
- We estimate that 450 MX and 30 Microfluorescence displaced NSLS users per year could be accommodated in an economically efficient manner
  - If all existing APS MX bending magnet beamlines were fully operational and staffed
  - Including minor improvements and additional staffing for a few insertion device beamlines

APS Life Sciences Bending Magnet Beamlines Status and Potential

- 14-BM-C BioCARS Operational; will be shut down if something major breaks
- 18-BM BioCAT Not built out
- 19-BM-D SBC-CAT Operational
- 21-BM LS-CAT Not built out
- 22-BM-D SER-CAT Operational
- 23-BM-B GM/CA@APS Operational
- 24-BM NE-CAT Enclosures are built, but hardware from 8-BM not assembled
- 31-BM LRL-CAT Not built out

Beamline	Current Techniques	Potential Techniques	Estimated Capacity Available (BL)	Estimated Capacity Available (Users/Year) *	One-time Costs for Increased Capacity (K$)	Recurring Costs for Increased Capacity (K$/Year)	Comments on Costs
8-BM	Micro-fluorescence	Micro-fluorescence	0.15	30	$75	125	KB mirror (cost share w/ BES) 0.5 Staff Scientist
14-BM-C	MX	MX	0.5	100	0	225	1.0 Staff Scientist
17-ID-B	MX	MX	0.15	30	0	125	0.5 Staff Scientist
19-BM-D	MX	MX	0.10	20	0	0	
22-ID/BM	MX	MX	0.25	50	$140	225	1.0 Staff Scientist to support remote access; Increased automounter capacity and sample visualization
23-BM-B	MX	MX	0.25	50	0	125	0.5 Staff Scientist
24-BM-B	Currently not operating	Life sciences	1	200	500	625	PSS, optics installation, controls/IT, 2 Staff Scientists and Scientific Assoc.
TOTAL			**2.4**	**480**	**715**	**1450**	

* Based on 200 users/beamline/year

New energy storage hub offers great opportunities for discovery, innovation, and impact

JCESR

Building a winning team

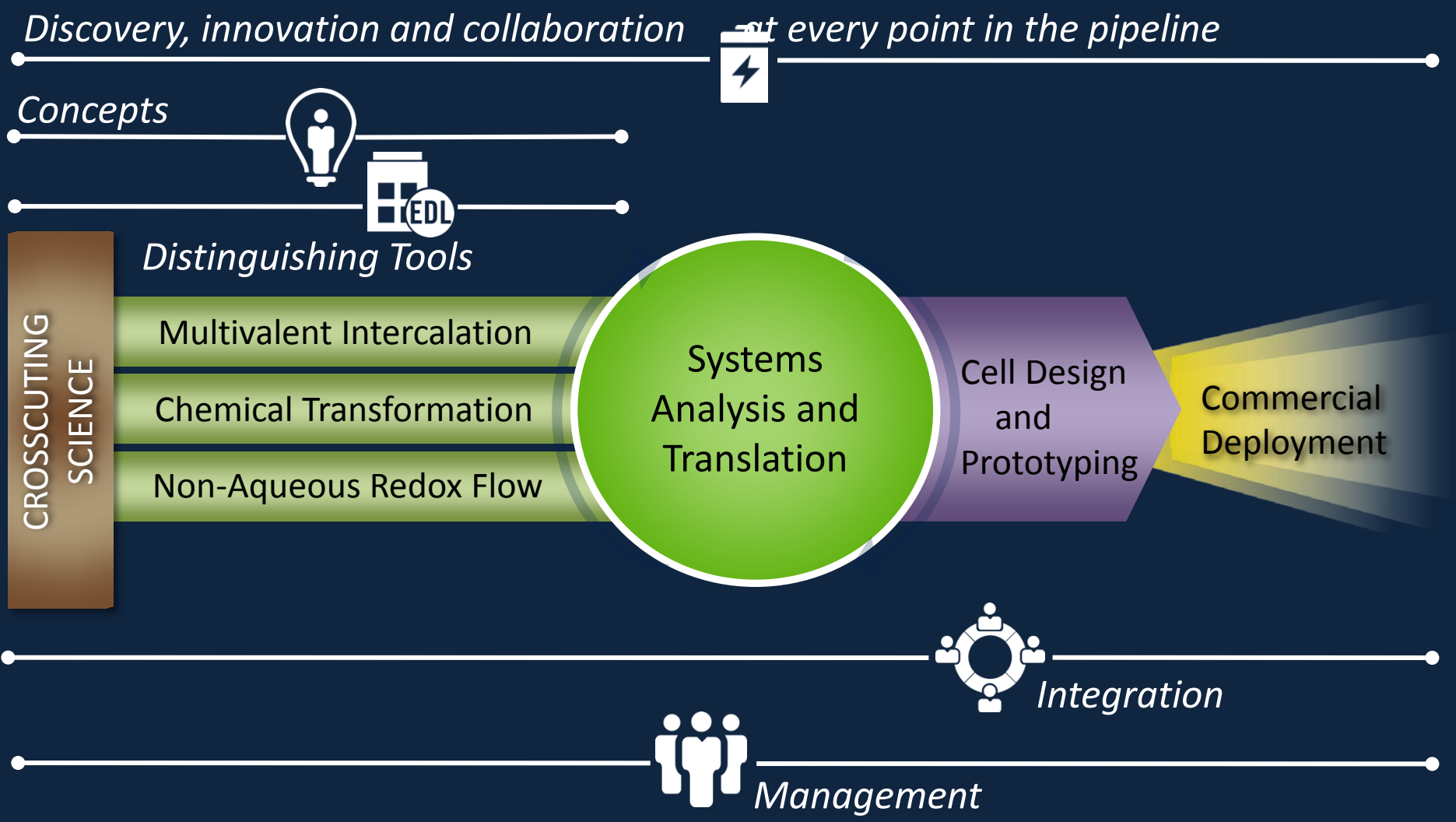
5
National Laboratories

5
Universities

4
Private-Sector Partners

Argonne NATIONAL LABORATORY
MICHIGAN
BERKELEY LAB
NORTHWESTERN UNIVERSITY
Dow
THE UNIVERSITY OF CHICAGO
JCESR
UIC UNIVERSITY OF ILLINOIS AT CHICAGO
APPLIED MATERIALS
ILLINOIS
+CLEAN ENERGY TRUST
SLAC NATIONAL ACCELERATOR LABORATORY
Johnson Controls
Pacific Northwest NATIONAL LABORATORY
Sandia National Laboratories

Building a new model of innovation



JCESR Impact: Achieving goals for lasting legacies

TRANSPORTATION

$100/kWh

400 Wh/kg **400** Wh/L

800 Wh/ **800** W/L

1000 cycles

80% DoD C/5

15-yr calendar life

EUCAR

GRID

$100/kWh

95% round-trip efficiency at C/5 rate

7000 cycles C/5

20-yr calendar life

Safety equivalent to a natural gas turbine

Legacies

- Pre-commercial prototypes for grid and transportation
- Library of fundamental knowledge
  - Atomic and molecular understanding of battery phenomena
- New paradigm of battery development
  - Science-based rational design
  - Systems-centric
  - End-to-end integration