APS Upgrade: Responding to BESAC call to address pressing research needs, assure U.S. global leadership

Maintaining U.S. position within the competitive landscape was a central theme in the July 2013 Report of the BESAC Subcommittee on Future X-ray Light Sources

- ‘…The Office of Basic Energy Sciences should ensure that U.S. storage ring x-ray sources **reclaim their world leadership position**…’

- “The very large, diverse U.S. user population presently utilizing U.S. storage rings represents a major national resource…It is **essential that the facilities** this science community relies on **remain internationally competitive** in the face of innovative developments… in other countries”

- ‘…developments include **diffraction limited storage rings with beamlines, optics and detectors** compatible with the $10^2 – 10^3$ increase in brightness…’

- ‘…recommendation for a new U.S. light source facility should not be based on capacity issues, but rather on **science-driven needs for new and unavailable photon characteristics** that would allow users to carry out previously impossible grand challenge experiments…’
The APS Upgrade: Building the world’s leading high-brightness hard x-ray synchrotron facility

The APS Upgrade is a next-generation facility:
- Optimized for hard x-rays
- Incorporating advanced beamlines, optics and detectors
- With ‘round’ source ideal for imaging

APS-U exceeds the capabilities of today’s storage rings by 2 to 3 orders of magnitude in brightness, coherent flux, nano-focused flux
- Increases coherent flux by x350 at 20 keV
- Extends coherence-based methods to 50 keV
- Serves very broad x-ray energy range: 0.25 keV to >150 keV

Powers the entire beamline suite to meet the needs of APS’ community of >5,000 unique users per year

World’s brightest storage ring light source above 4 keV
APS Upgrade design concept and scope

- New storage ring optimized for low emittance and high-brightness
  - 6 GeV MBA lattice (with 2x current) in existing tunnel
- New insertion devices optimized for brightness and flux
  - Superconducting undulators on selected beamlines
  - New and upgraded ID front-ends of common design; higher power and maximum flexibility
- Beamlines
  - Suite of six new and two heavily-upgraded beamlines designed for best-in-class performance with high-brightness source
  - Optics/stability/detector improvements for remaining beamlines, assuring that all beamlines take full advantage of MBA source properties
  - More than 60 operating beamlines at project completion, all with improved performance

The APS Upgrade Concept fulfills the BESAC vision: To build the world’s leading high-brightness hard x-ray storage-ring user facility
APS Upgrade multi-bend achromat lattice concept

\[ \varepsilon_x = C_L \frac{E^2}{N_D^3} \]

\( E = \) Beam energy (\( E = 6 \) GeV for APS MBA)
\( N_D = \) Number of dipoles per sector (\( N_D = 7 \) for APS MBA)

~50-fold reduction in horizontal emittance

– J. Murphy, BNL-42333
APS Upgrade ensures that the United States maintains world leadership in light sources

Curves for APS, ESRF and SP8 upgrades based on present designs, assuming identical undulators
APS-U: The ultimate 3D microscope

A new analytical tool to approach the supreme goal of measurement science:
To map any atom’s position, identity and dynamics

- **High Energy**
  - Penetrating bulk materials and operating systems
    - World’s brightest source of hard X-rays
    - 3D mapping, deep inside samples
    - X-ray cinematography in previously inaccessible regimes

- **Brightness**
  - Providing macroscopic fields of view with nm-scale resolution
    - Multi-scale imaging – connecting nanometer features across macroscopic dimensions
    - Fast sampling with chemical, magnetic, electronic sensitivity

- **Coherence**
  - Enabling highest spatial resolution even in non-periodic materials
    - Extends lensless imaging to hard x-ray domain, with resolution down to <1 nm, localizing atoms
    - Increases phase contrast for fast full field imaging
    - Correlation methods improve by 10,000-1,000,000x

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- **CuAsW**: 100 nm

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- **Steel Cylinder**: Pre-shot image
- **100 nm**: CuAsW

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Penetrating bulk materials and operating systems

Providing macroscopic fields of view with nm-scale resolution

Enabling highest spatial resolution even in non-periodic materials

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The APS Upgrade’s well-honed science case has been developed by a diverse community of users over a decade

- Science case based on sustained, decade-long community-based effort
- APS-U Early Science document articulates compelling scientific vision
  - Reflects input from hundreds of researchers worldwide
  - Report based on series of multi-disciplinary science planning workshops

- Early Science expresses the priorities outlined in the recent BESAC report:
  ‘Whether the application is data storage, aircraft turbine blade design, advanced catalysts, combustion science, drug delivery, computers, structural materials, or medical implants, 4D maps of matter … are essential to quantitative prediction of materials properties and behavior.’
  – Challenges at the Frontiers of Matter and Energy
Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

‘Advances in imaging capabilities provide an opportunity to expand our ability to observe and study matter from the 3D spatial perspectives of today to true ‘4D’ spatially and temporally resolved maps of dynamics that allow quantitative predictions of time-dependent material properties and chemical processes.’

– Challenges at the Frontiers of Matter and Energy

APS-U’s **game-changing coherence and brightness** deliver precisely the **advanced multimodal imaging** and measurement capabilities outlined by BESAC:

- Map all of the critical atoms in a cubic millimeter, bridging lengthscales from atoms to nanostructure
- Probe grains deep within real materials under realistic conditions
- Sample vast regions of experimental phase space with sufficient time resolution to capture rare events
- Image heterogeneous materials and interfaces, linking molecular to mesoscale phenomena

*With APS-U: 1 nm catalytic nanoparticles clearly visible on alumina surface*
Transformative Opportunity

Mastering Hierarchical Architectures and Beyond-Equilibrium Matter

‘The emergent functionalities enabling next-generation disruptive energy technologies require mastering the design, synthesis, and control of complex hierarchical materials employing dynamic far-from-equilibrium behavior.’

– Challenges at the Frontiers of Matter and Energy

APS-U’s brightness and high-energy penetrating x-rays will enable measurements at spatial and time resolutions and under conditions that are inaccessible today

- Probing materials, devices and chemical processes in situ and operando
- Real-time observation of architecture and development in hierarchical materials
  – Imaging structure and dynamics during materials synthesis
- Fast imaging at high resolution across lengthscales
- Experiments validating and verifying predictive models
Finding the ‘missing’ zeolites

Structure direction in the assembly of zeolites

APS-U enables development of tailored catalytic materials and sites; offers x-ray fluctuation microscopy to probe ordering from sub-nm to microns during assembly

Structure dynamics during materials synthesis

Simulated APS-U time-time correlation functions during layer-by-layer crystal growth, for differing adatom transport regimes

Hierarchical imaging of complex systems

Map the finest cellular processes of neurons and their connections across the brain: ‘connectomics’

APS-U enables 3D visualization with unprecedented detail; e.g., ptychography across ~1 mm$^3$ at ~10nm resolution in a few days vs. > a year today
Beyond Ideal Materials and Systems: Understanding Critical Roles of Heterogeneity, Interfaces and Disorder

‘Expanding our scientific knowledge from the relative simplicity of ideal, perfectly ordered, or structurally averaged materials to the true complexity of real-world heterogeneities, interfaces, and disorder should enable us to realize enormous benefits in the materials and chemical sciences…’

– Challenges at the Frontiers of Matter and Energy

APS-U’s greatly increased flux of spatially coherent x-rays will provide unprecedented understanding of nm-scale heterogeneity:

- Thorough multi-scale studies of heterogeneous populations at timescales ranging from tens of picoseconds to days
- Advanced coherent imaging techniques providing quantitative 3D images of defects, disordered materials and heterogeneous bulk materials
- Imaging heterogeneous materials and interfaces in natural systems, linking molecular to mesoscale transport phenomena
- Probing in situ multiscale structure in heterogeneous systems at high energies
  - Essential for catalysts, batteries, geological materials, shale dynamics, and nanoelectronics
Transformative Opportunity

Beyond Ideal Materials and Systems: Understanding Critical Roles of Heterogeneity, Interfaces and Disorder

Atomic-scale physics of amorphous metals

Simulated difference in coherent scattering patterns before and after yielding event in amorphous metal

Few- to 100-atom shear transformation zones (STZ) hypothesized to underlie plasticity, failure

Unprecedented opportunity for 3D atomic reconstructions

Developing new, more durable structural materials

State of the art today: 1 μm 2D focus to study 30 μm grains

With APS-U, twin bands and initial crack are resolved

With APS-U: 80 keV brightness to penetrate bulk materials, measure strains with 100nm resolution

APS-U enables coherent imaging to measure intragrain and grain boundary properties

Single-defect imaging: defects as key system components

Simulated reconstruction of nanocrystal with atomic vacancies, using Bragg coherent diffraction imaging

APS-U will achieve the ultimate structural resolution in situ
Harnessing Coherence in Light and Matter

‘The ability to implement full control of large-scale quantum-coherent systems has the potential to advance the frontiers of chemistry and physics and to revolutionize technology in areas such as information processing, sensor technology, and energy generation/transformation.’

– Challenges at the Frontiers of Matter and Energy

APS-U will offer capabilities anchored by enhanced coherent x-ray flux and high photon energy that will open new windows on emergent phenomena in condensed matter physics

- Unique opportunities to study tuned quantum phase transitions, e.g. by pressure or magnetic field
- Picosecond time resolution ideal for pump-probe coherent phenomena in condensed matter experiments
- High-energy x-rays are required to probe excitation in heavy elements systems (e.g. iridates)
Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing

Tremendous synergies exist between the computational needs of the APS-U and ongoing national investments in Argonne’s computational resources and research.

Argonne’s planned exascale computational resources are critical to realization of APS-U’s full scientific potential:

- Adaptive control of experiments to ‘zoom in’ on unusual regions or rare events
- On-demand access to high-performance computing will provide near-real-time data feedback to users
- Interpretation and visualization of large, complex data streams beyond unaided human comprehension
- Combined simulations and multimodal data to address currently intractable scientific problems
- Automated cataloging, transport, and reduction of data streams of petabytes/day/beamline

Integration of APS/ALCF continues to strengthen:

- Terabit networking between ALCF and APS
- Real-time analysis; new methods, applications, software
APS Upgrade cost estimate is well established

Cost has been thoroughly vetted, compares favorably with recent project experience

- APS-U cost estimate presented at CD-1 Review: TPC = $734M
  - Based on assumed funding profile and project schedule
  - TPC includes costs associated with the previous version of Upgrade and 33% contingency on cost-to-go, consistent with project status
  - Leverages existing APS infrastructure, valued at ~ $1.5 billion
- APS-U has been funded at $20M/year for FY12-16
  - Costed and committed ~$83M
- APS-U cost estimate will be revised to include LDRD assessment (~$33M), funding profile adjustments, and incorporate beamline planning outcomes

APS-U Total Project Cost breakdown including contingency ($M)

- Accelerator, $343.6
- Previous Scope (U1), $43.9
- Project Management, $52.7
- Beamlines, $196.1
- Front-end and IDs, $97.6
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- Project Management, $52.7
- Beamlines, $196.1
- Front-end and IDs, $97.6
- Cost has been thoroughly vetted, compares favorably with recent project experience
Beamline planning process complete in summer 2016
Upon completion, APS-U will power a full suite of more than 60 beamlines

APS-U Project scope includes
- 8 newly constructed/upgraded world-leading beamlines
- Performance enhancements to nearly all remaining beamlines

Recent call for new/upgraded beamline proposals drew 36 whitepapers from physical, environmental, life sciences and engineering
- Diverse proposals exploit APS-U’s high energy, coherence-based techniques, micro/nano-focusing
- Imaging studies over many lengthscales; including multimodal techniques
- Dynamics and real-time studies; multi-timescale scattering/spectroscopy/imaging
- Multiple in situ and operando approaches
Final beamline selection expected July 2016

APS-U Experimental Capabilities

- Highest resolution hard x-ray scanning probe imaging, down to 5 nm (20 nm in complex in situ/operando environments)
- Ptychography and coherent imaging with spatial resolutions down to the localization of single atoms, as well as ability to follow dynamic processes in close to real time
- High energy, highest resolution 3D imaging, down to 100 nm at 80 keV
- Extension of coherence techniques to high energies; combined ptychography with HE diffraction microscopy, yielding local ~10 nm resolution in global fields of view
- Trace element sensitivity to below 10 atoms
- X-ray photon correlation spectroscopy down to 10s of ns correlation times, and higher order spectroscopies
- High-pressure science at TPa and high temperature, with 10-nm sensitivity
At end of one-year installation shutdown, APS-U will boast full complement of 60-plus beamlines optimized to exploit new source capabilities and to meet scientific needs of our >5,000-member user community.
APS Upgrade’s leadership team is complete and ready to deliver this project successfully

APS-U is managed by a strong team with extensive project experience; Technical managers bring deep experience from original APS construction
APS Upgrade’s leadership team is complete and ready to deliver this project successfully.

APS-U is managed by a strong team with extensive project experience; Technical managers bring deep experience from original APS construction.
APS-U technical and project plans have been vetted by dozens of external experts in >20 reviews

APS-U has a robust advisory committee structure, made up of internationally recognized experts:

**Machine Advisory Committee (MAC):** Robert Hettel (SLAC), chair

**Experimental Systems Advisory Committee (ESAC):** Piero Pianetta (SLAC), chair

**Project Management Advisory Committee (PMAC):** Carl Strawbridge (High Bridge Consultants), chair

- APS-U has vetted plans in 20 reviews and advisory committee meetings over the last two years:
  - Technical: 11 design reviews; two integrated conceptual design reviews (MAC and ESAC)
  - Management: Two project management advisory committee reviews
  - Cost and schedule: Five deep-dive cost/schedule reviews

- Integrated CD-1 Readiness Review (Director’s Review): 21 external experts covering technical, management, cost and schedule, safety

- To prepare for the next step, APS-U is planning a series of ~10 preliminary design reviews over the next six months

- Planning under way for next set of science workshops
Two recent major DOE reviews have validated APS-U Project readiness for Critical Decision 1

DOE/SC review of APS-U (Sept. 22-24, 2015)

- ‘…the project is ready for CD-1 approval. The conceptual design for the new storage ring is sound…’
- ‘…the planning and R&D are well advanced for this stage of the project.’
- ‘…the project documentation is in good shape for CD-1…the point estimate for the TPC is reasonable…’
- ‘…the APS-U project management team is strong, capable, motivated, and fully engaged.’
- The project has met all of the prerequisite requirements, and the project is ready for CD-1.’


- ‘The project team cost estimate is high quality and includes detailed backup documentation and good application of models… The ICR team recommends approval of the APS-U for CD-1…’

APS-U CD-1 was approved February 4, 2016
Advanced Photon Source Upgrade
At Argonne National Laboratory
CD-1 Refresh ESAAB – Equivalent Review

Approval:

Based on the information presented above and at this review, Critical Decision-1 Refresh,
Approve Revised Cost Range is approved and authorized to proceed with the preliminary design
and planning, establishing the performance baselines for the Advanced Photon Source Upgrade
project.

Franklin M. Orr, Jr., Project Management Executive
Under Secretary for Science and Energy

2/4/16
Date
APS-U R&D, prototyping are progressing at a strong pace
To stand still is to lose ground

Our plans for the APS Upgrade enable the U.S. to maintain a world leadership position in storage ring-based x-ray sources – but success depends on timely completion.

**ESRF (France)** – 2nd phase of upgrade incorporates MBA lattice; plans to resume operation in 2020, complete 4 state-of-the-art beamlines by 2022

**SIRIUS (Brazil)** – Completing final design; operational in 2018

**MAX-IV (Sweden)** – Construction underway; inauguration June 2016

**SPRING-8 (Japan)** – Capable of upgrading in 2020 timeframe

**HEPS (China)** – Greenfield accelerator facility to be built near Beijing; planned completion in early 2020s

**APS-U** – Resume operation in 2022
APS-U: The world’s leading hard x-ray lightsource addressing the grand challenges of this century

APSU is uniquely positioned to provide the high energy, brightness, and coherence required to address the transformational opportunities posed by BESAC – and to support world-leading science for decades to come.

APS-U is ready to proceed to construction
- The concept is sound and well-vetted
- R&D is moving forward at a strong pace, proving that the technical challenges can be met
- Cost is well-understood and based on solid estimates and comparisons
- A strong, experienced project team is in place and moving forward
- The community is enthusiastic and supportive of the APS-U plans

Timeliness is of the essence to meet foreign competition and sustain U.S. leadership in high-energy x-ray science
Backup Slides
The world's six leading storage rings in 2021 – without APS Upgrade

- **MAX-IV**
  - Lund, Sweden
  - 2016
  - 528m

- **Petra III**
  - Hamburg, Germany
  - 2012
  - 2,300m

- **HEPS**
  - Beijing, China
  - 2021
  - ~1,300m

- **ESRF (UPGRADE)**
  - Grenoble, France
  - 2020
  - 844m

- **SIRIUS**
  - Campinas, Brazil
  - 2018
  - 518m

- **SPRING-8 (UPGRADE)**
  - Harima, Japan
  - 2020?
  - 1,436m
APS-U will serve a large, active and growing user community

- >28,000 participations, >5000 unique onsite and offsite users in FY14
- >5700 experiments; > 1800 publications in 2014
- > 200 (unique) industrial users in FY14 from pharma, energy, electronics, materials

**APS serves more users than any other DOE Scientific User Facility**
The community is enthusiastic about the APS Upgrade plans

- > 200 participants in the most recent workshop series
- Early Science report has 115 authors from 49 Institutions

The recent beamline proposal solicitation resulted in

- 36 Proposals, with 215 unique investigators from 91 Institutions including universities, industries and laboratories
- These proposals represent a stakeholder community including > 200 institutions
APS Upgrade provides exceptional hard x-ray brightness among domestic sources

Brightness vs. x-ray energy at top beamlines among BES synchrotron facilities
Comparison of APS-U to other light sources worldwide in early 2020s

<table>
<thead>
<tr>
<th>Parameter</th>
<th>APS Present</th>
<th>APS Upgrade</th>
<th>ESRF-II</th>
<th>SPring8-II</th>
<th>Petra-III</th>
<th>NSLS-II</th>
<th>MAX-IV</th>
<th>Sirius</th>
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<td>6</td>
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<td>6</td>
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<td>99</td>
<td>1000</td>
<td>800</td>
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<td>Brightness (*)</td>
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<td>8 keV</td>
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<td>88</td>
<td>61</td>
<td>43</td>
<td>4.1</td>
<td>3.7</td>
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<td>137</td>
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<td>382</td>
<td>154</td>
<td>127</td>
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<td>Flux Density (*) (#)</td>
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<td>8 keV</td>
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<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
<td>1.8</td>
<td>0.4</td>
<td>2.0</td>
<td>1.7</td>
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<td>20 keV</td>
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<td>10.4</td>
<td>7.7</td>
<td>4.1</td>
<td>1.4</td>
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<td>0.6</td>
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<td>80 keV</td>
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<td>10.4</td>
<td>7.5</td>
<td>3.9</td>
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<td>Coherent Flux (10^{11} ph/s)</td>
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<td>8 keV</td>
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<td>813</td>
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<td>398</td>
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<tr>
<td>Single Bunch Brightness @ 8 keV (*)</td>
<td>1</td>
<td>25.5^{(&amp;)}</td>
<td>1.5</td>
<td>5.1</td>
<td>0.3</td>
<td>0.1</td>
<td>1.9</td>
<td>3.1</td>
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<tr>
<td>Flux for 10 nm focus @ 8 keV (*)</td>
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<td>88</td>
<td>61</td>
<td>43</td>
<td>4</td>
<td>4</td>
<td>14</td>
<td>23</td>
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</table>

(*) Relative to present APS performance
(#) Flux Density is through a 0.5 x 0.5 mm aperture at 30 m
(&) APS-U 48 bunch timing mode

No light source now operating, under construction or planned can match all of APS-U’s technical capabilities
APS-U removal and installation plan

- Minimizing APS unavailability with a well-defined installation period is a key deliverable of the APS Upgrade Project.
- The Project has developed and has independently reviewed a bottom-up 12 month plan for removal, installation, and testing-with-beam for the facility.
- Plan has substantial detail for this stage of the Project
  - Multi-shift (two shifts initially, 5 days/week)
  - Multi-crew operation; each responsible for 6-8 sectors
  - Material removal ~ 1800 tons, Material installation ~ 3000 tons
  - 131 FTE over 9 months of storage ring removal and installation: Approximately 1/3 trades; 1/3 term ANL; 1/3 permanent ANL
- Risk mitigation includes additional shifts, additional workdays

<table>
<thead>
<tr>
<th>TASK</th>
<th>Month 1</th>
<th>Month 2</th>
<th>Month 3</th>
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<th>Month 6</th>
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<th>Month 10</th>
<th>Month 11</th>
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<td>Accelerator Readiness Review</td>
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<td>Testing with Beam</td>
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</table>
Removal and Installation

- Comparisons have been drawn with the actual transition periods of past machines, and plans of future facilities.
- The Project, and our reviewers, find our plan credible.

<table>
<thead>
<tr>
<th>Light Source</th>
<th>SR Circum. (m)</th>
<th>Remove Duration</th>
<th>Install Duration</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSRL/SPEAR3</td>
<td>234</td>
<td>5 weeks</td>
<td>27 weeks</td>
<td>Similar scope to APSU (1/5 length), Complete ring replacement, 1 access point</td>
</tr>
<tr>
<td>NSLS II</td>
<td>792</td>
<td>N/A</td>
<td>128 weeks</td>
<td>Limited by equipment availability</td>
</tr>
<tr>
<td>PETRA III</td>
<td>2304</td>
<td>~12 weeks</td>
<td>~24 weeks</td>
<td>1/8 of 2304 m ring removed and replaced (~300 m)</td>
</tr>
<tr>
<td>ESRF II</td>
<td>844</td>
<td></td>
<td>48 weeks</td>
<td>Planned; 20 months stop to start for user operations</td>
</tr>
<tr>
<td>MAX IV</td>
<td>528</td>
<td>N/A</td>
<td>52 weeks</td>
<td>Planned</td>
</tr>
<tr>
<td>Pohang</td>
<td>282</td>
<td>12 weeks</td>
<td>12 weeks</td>
<td>Complete; 6 month commissioning</td>
</tr>
<tr>
<td>APS-U</td>
<td>1104</td>
<td>8 weeks</td>
<td>28 weeks</td>
<td>Planned; 5 access points</td>
</tr>
</tbody>
</table>