PRESENTED TO BESAC
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APS-U PROJECT UPDATE AND SCIENTIFIC IMPACT

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BES' LIGHT SOURCE STRATEGY

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*

- *"…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** …."*
- *"…The Office of Basic Energy Sciences should ensure that U.S. storage ring x-ray sources **reclaim their world leadership position**…"*
- *"…developments include **diffraction limited storage rings with beamlines, optics and detectors** compatible with the 10^2 – 10^3 increase in brightness…"*
- *"…an exciting window of opportunity exists for the U.S. to provide a revolutionary advance in X-ray science by developing and constructing an unprecedented X-ray light source. This new light source should provide **high repetition rate, ultra-bright, transform limited, femtosecond X-ray pulses over a broad photon energy range** with full spatial and temporal coherence."*

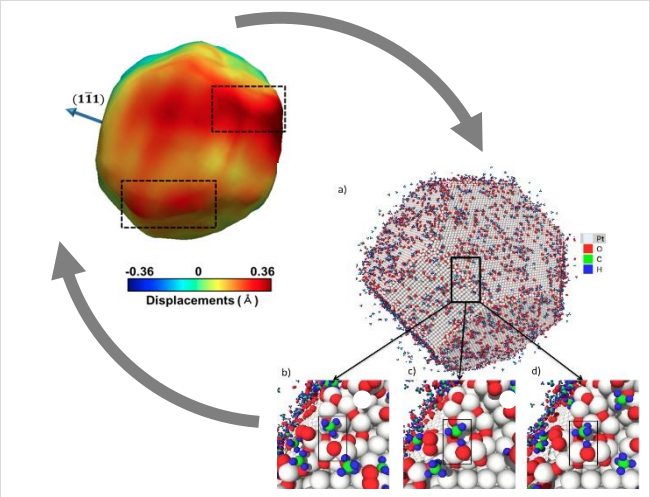
THE APS UPGRADE

OUTCOME

By 2026, the world's leading hard x-ray microscope — the upgraded APS — will enable multiscale, three-dimensional exploration of complex materials and chemical systems in unprecedented detail

SIGNIFICANCE

APS-U will provide unique tools for understanding materials and chemical systems under operational conditions and at the atomic scale



Platinum nanoparticle in a catalytic environment: coherent diffractive image (left) and molecular dynamics simulation (right)

APS-U

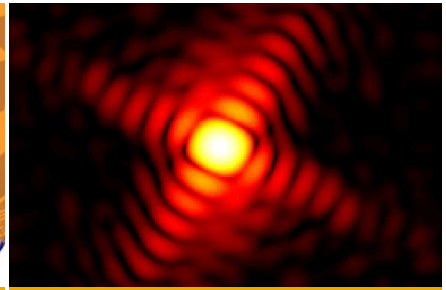
A new analytical tool to approach the supreme goal of measurement science: to map any atom's position, identity, and dynamics

High Energy

Penetrating bulk materials and operating systems

Brightness

Providing macroscopic 3D fields of view with nm-scale resolution



Coherence

Enabling highest spatial resolution even in non-periodic materials

Complementary to other DOE light sources

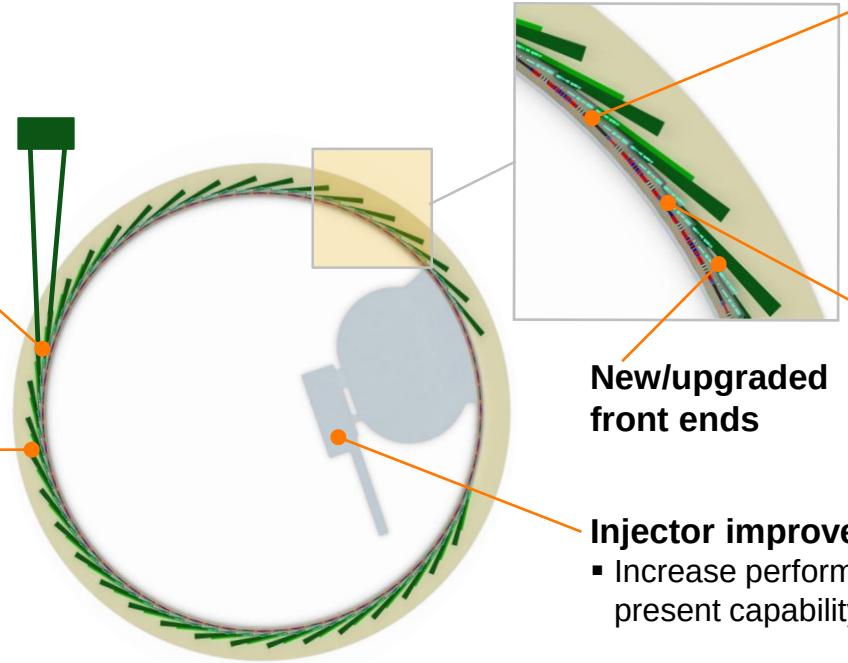
- NSLS-II
- SSRL
- ALS-U
- LCLS-II(-HE)

APS UPGRADE PROJECT SCOPE

Maximize scientific capability

Feature beamlines
- Suite of beamlines, including long beamlines, designed for best-in-class performance

Beamline enhancements
- Improvements to make beamlines “Upgrade Ready”
- Existing beamlines are planned to come back on-line after the upgrade



New storage ring
- 6 GeV with 200 mA, 42 pm-rad emittance
- Hybrid 7BA lattice with reverse bends
- Improved electron and photon stability

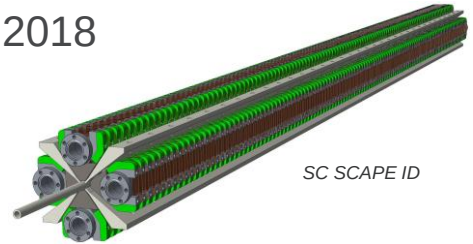
New/upgraded front ends

New insertion devices
- Including superconducting undulators

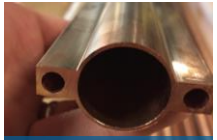
Injector improvements
- Increase performance beyond present capability

APS UPGRADE STATUS

- Storage ring hardware development phase is drawing to a close and detailed designs for all systems are in full swing
- Beam physics and lattice design were independently reviewed and confirmed in May 2018
- Execution of ~$42M of CD-3B authorized LLPs for storage ring, front ends, insertion devices, and beamlines is underway
- CD-2 Review will take place in October 2018
- Earliest first light in 2023, CD-4 in FY26



SC SCAPE ID



Cu chamber extrusion; to be NEG-coated

Velociprobe for rapid scan nanoprobe

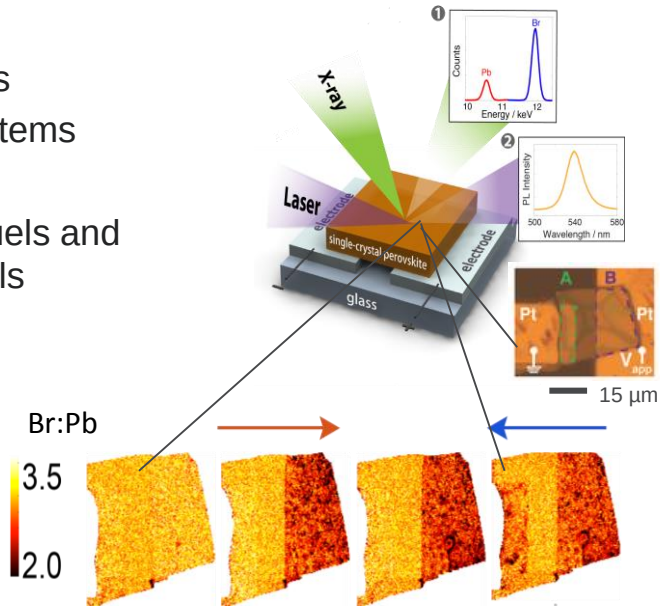
Storage Ring Vacuum System Test Sector

First APS-U production magnet

IN SITU AND OPERANDO STUDIES OF DEFECTS

Development of advanced materials requires understanding of defect dynamics (including interfaces) during processing and operation

- Quantum systems
- Energy-water systems
- Nano-electronics
- Nuclear energy fuels and structural materials



X-ray & luminescence imaging show Br and Pb ion migration under applied voltage.

Br distribution never fully recovers, even under reverse bias.

Y. Luo et. al, *Adv. Mater.* **29**, 1703451 (2017).

MULTIMODAL CHARACTERIZATION

- *Operando* studies of transport behavior,chemical reactions, and optoelectronic phenomema in novel materials

FUTURE

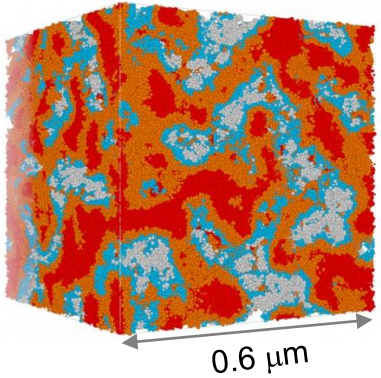
- 10x increased resolution enables probing of single defects
- 1000x increased flux enables fast tracking of metastable intermediates and crystallization during growth, and the ability to capture rare events
- Broad *in-situ* capabilities enable deeper understanding of material evolution during processing

TRANSPORT AND DYNAMICS IN NANOSCALE NETWORKS

APS-U enables imaging across nano- and mesoscales

EXAMPLE PROBLEM

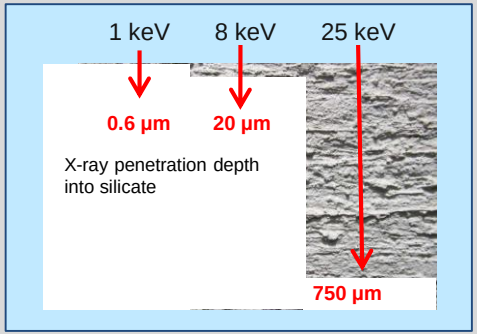
- Nanoscale pore spaces play a major role in properties of silicate composites, e.g. during water freeze/thaw
- Can now simulate calcium silicate hydrate on micron-size scales
- **But** can NOT effectively characterize 1-20 nm pore networks across relevant 3D field of view, because adequate tools with both high resolution and extended 3D field of view are ***not available today***



Simulated calcium silicate hydrate (C-S-H) : K. Ioannidou et al, PNAS, 2016. 113 (8) 2029-2034

APS-U will make it possible to determine structure and chemical composition at nanoscale resolution matched to pore network, in relevant sample volumes

- **Structural materials, including concrete**
- **Electrochemical systems**
- **Soil networks, other environmental systems**
- **Cells and other biological systems**

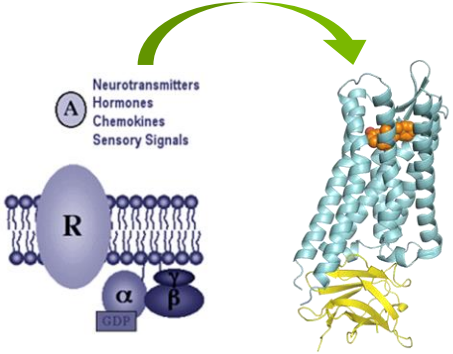


ACCELERATING STRUCTURE BASED DRUG DESIGN AND DISCOVERY

Drug discovery is slow and extremely costly

Opioid (pain killer) crisis:
μ-opioid receptor

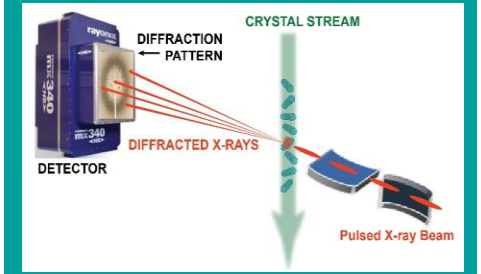
G-protein coupled receptors are the largest class of pharmaceutical targets



Model from biochemical interpretation

μ Opioid receptor in the active state with a morphinan agonist bound

APS-U enables high-throughput structure determination up to 1,000's of structures per day



Drug development at APS

Januvia
diabetes, Merck

Kaletra
HIV, AbbVie

Votrient
kidney cancer, GlaxoSmithKline

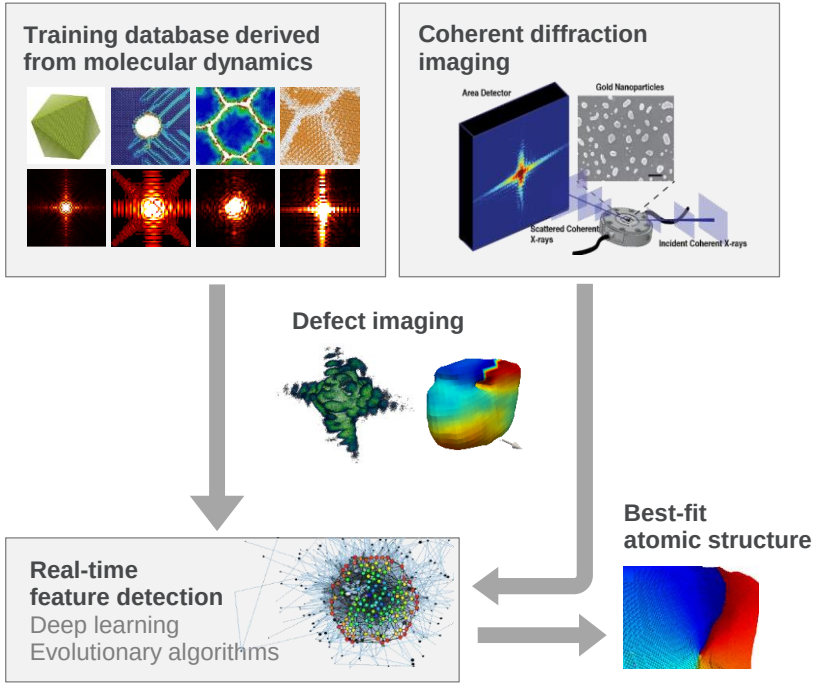
Zelboraf
melanoma, Genentech

Venclexta *leukemia, AbbVie*

X-RAYS AND ARTIFICIAL INTELLIGENCE

Combining coherent imaging, simulation, and deep learning

- **A single APS beamline can currently produce 200TB/day**
- **Expected to produce 10-100PB/day raw data in 10 years**
- **Single Reconstruction:**
  - Today: 512 x 512 x 512 volume elements
    - 30 gigabytes (for phasing)
    - 7nm resolution
  - APS-U: 5120 x 5120 x 5120 volume elements
    - 30 terabytes (for phasing)
    - 7Å resolution



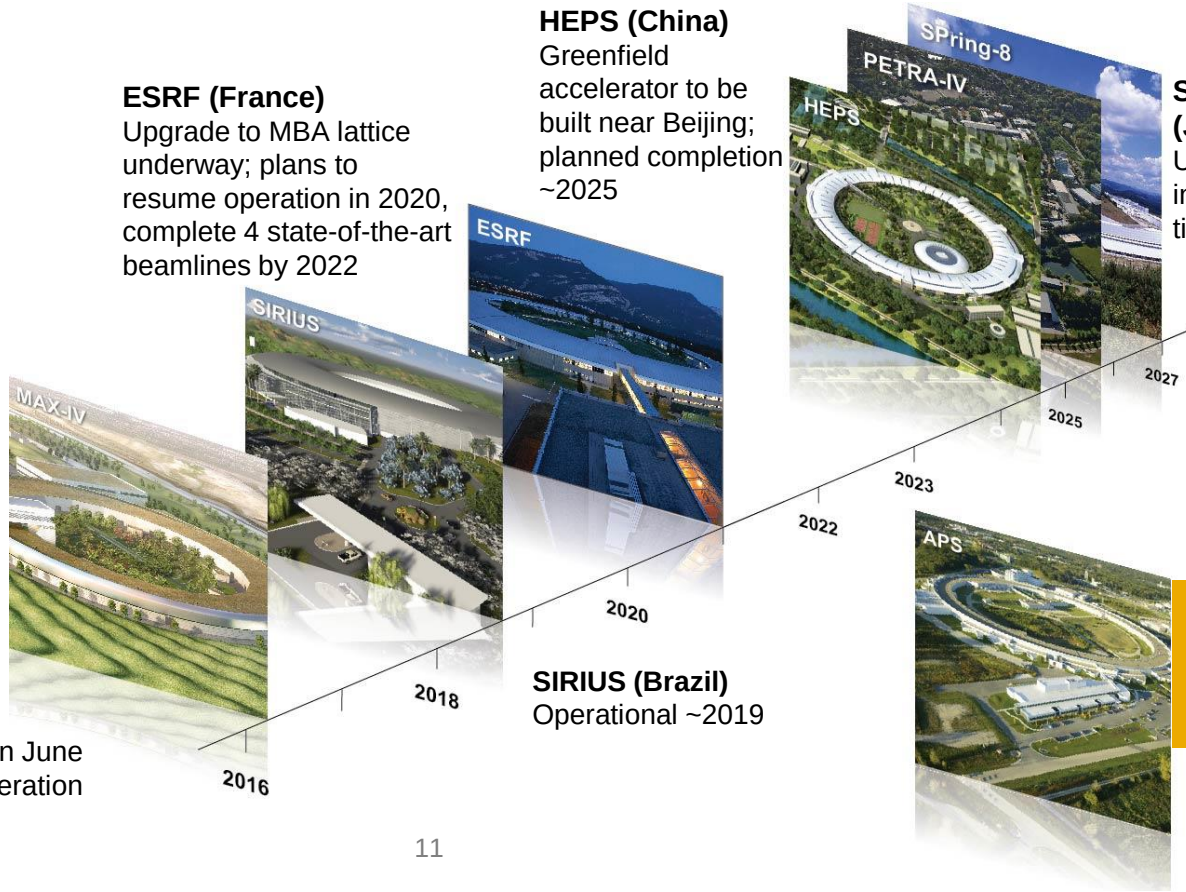
TO STAND STILL IS TO LOSE GROUND

Our plans for the APS Upgrade maintain world leadership in storage ring-based x-ray sources

ESRF (France)
Upgrade to MBA lattice underway; plans to resume operation in 2020, complete 4 state-of-the-art beamlines by 2022

HEPS (China)
Greenfield accelerator to be built near Beijing; planned completion ~2025

SPring-8 (Japan)
Upgrading in 2027 timeframe



MAX-IV (Sweden)
Inauguration June 2016; in operation

SIRIUS (Brazil)
Operational ~2019

APS-U
Resume operation in 2023

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