ALS User Forum on the ALS-U Project Beamlines

February 25, 2019
Agenda

• **ALS-U beamline selection process and the path to ALS renewal**
  – David Robin (ALS-U Project Director)
  – Andreas Scholl (Interim ALS Science Deputy)

• **Science at the new and upgraded ID beamlines**
  – COSMIC upgrade, David Shapiro (ALS) and Will Chueh (Stanford)
  – MAESTRO upgrade, Eli Rotenberg (ALS) and Jyoti Katoch (Carnegie Mellon)
  – New tender x-ray beamline, Chenhui Zhu (ALS) and Pupa Gilbert (University of Wisconsin–Madison)
  – New soft x-ray beamline, Sujoy Roy (ALS) and Alex Frano (UCSD)

• **Q&A**
ALS-U: Enabling the ALS’s global leadership in soft x-ray science

Features

• World-leading soft x-ray brightness and capabilities
• More than 100x increase in soft x-ray brightness and coherent flux compared with today’s ALS
• Excellent IR and hard x-ray capabilities

Impact

• Enable scientific advances in a diverse range of fields, improving our economy, healthcare, and national security
• Continue the ALS tradition of serving a large and scientifically diverse user community
The ALS today has...

- LINAC
- Booster ring
- Storage ring, featuring triple-bend achromat lattice
- 40 beamlines

Thin, wide electron beam profile
During the construction phase of the project...

The storage ring will be removed...

But the LINAC and booster ring will remain

And most of the beamlines will stay
During the construction phase of the project...

A new storage ring will be built, based on a 9-bend achromat.

And a second concentric "accumulator" ring will be added.

Bend and superbend beamlines will be realigned.

Some new insertion devices will be added to the ring.

A small number of new soft x-ray insertion-device beamlines will be added.

And a small number of soft x-ray insertion-device beamlines will be upgraded.

ALS-U Beamline Selection Process

= beamline included in ALS-U project
User community engagement in ALS-U beamline planning

Workshops

- Oct. 2014

User Meetings

- Jan. 2017

User Forums

- Topical Cross-Cutting Reviews & Workshops
- Web Forms
- Informal Conversations
Examples of community input

• “Current-day RIXS experiments will highly profit from the smaller beam provided by ALS-U since it enables a smaller spot size on the sample...”

• “...developing a technique capable of simultaneously probing multiple order parameters...and with spatial resolution for inhomogeneous sample would lead to major advances in the understanding and development of new materials.”
Prioritization criteria

- Scientific importance
- Relevance of ALS-U characteristics and potential world leadership
- Strength of the relevant user community and expected productivity
- Overall approach, feasibility, R&D activities, and fit to project resources
Decision-making process

• 16-month process
• User community and ALS staff input was evaluated, then synthesized into several beamline scenarios by a working group of ALS staff
• External committees (ALS and ALS-U advisory committees, a steering committee, and an ad-hoc evaluation committee) reviewed the scenarios
• Ad-hoc committee made a recommendation
• ALS-U Project Director made the final decision
ALS-U upgraded and new beamlines at the ALS

**Sector 7:** Upgrade MAESTRO and COSMIC (COSMIC XPCS to move to Sector 10)

**Sector 8:** Build a new tender x-ray beamline featuring STXM and coherent scattering

**Sector 10:** Build a new soft x-ray beamline featuring XPCS, nRSoXS, and nRIXS
Technique toolbox of the upgraded ALS
The capabilities imparted by the ALS-U project will provide the foundation for new ALS science.
Crosscutting challenges addressed by the future ALS

Spectral Mapping of Nano-Objects

Designing Functional Interfaces

Harnessing Entropy for Material and Chemical Design

Measuring & Manipulating Nanoscale Currents & Flows

Materials Chemistry and Physics in Confined Spaces
The ALS-U Project is independent of ALS.

Throughout the project and beyond, the ALS will continue to innovate with new and upgraded experimental systems, many of which will benefit from characteristics provided by ALS-U.

The input and advice we receive throughout the ALS-U Project will help inform ALS strategic planning and future projects.
COSMIC beamline upgrade

David Shapiro  
Advanced Light Source

Will Chueh  
Stanford University
COSMIC upgrade

**Existing layout**

**Upgraded layout (draft)**

**Current properties**

- Separate XPCS / STXM branches
- 250–2500 eV
- Resolving power: 3,000

**Upgrade scope**

- XPCS branch relocated to FLEXON
- Two STXMs share single branch
- Optical layout re-optimized
COSMIC: Spectro-Microscopy and Tomography of Functional Nano-Materials

- Chemical contrast: C→S K-edge
- Magnetization contrast
- Bond orientation contrast
- Ptychography: 3 nm resolution
- Cryogenic tomography
- Liquid, gas, heating, biasing samples

Nanoscale Magnetic Structures and Dynamics
- STXM
- Ptychography

Operando and Correlative Imaging of Materials
- Diffraction limited beamline optics, 15X higher coherent flux
- Single-nm spatial resolution, few microsecond time resolution
Addressing “Meso-time” Gap for Energy Materials

- Materials
  - Nanomaterials design
  - Spectroscopy, scattering & diffraction
  - Molecular Dynamics
- Devices
  - Phase Field
  - Microscopy
  - Tomography
- Systems
  - Data-driven models & analytics
  - Synthesis & fabrication
  - Characterization
  - Modeling & analytics
In-situ spectro-ptychography for investigating redox

Opportunities

• Significantly enhanced spatial/temporal resolution to reach the meso-time gap

• Understand redox reactions at the nanoscale

Challenges

• Sample damage, especially in liquid

• Data processing of sequential ptychography frames


Lim, Yu, Chueh, Shapiro et al. *In preparation*. 
MAESTRO beamline upgrade

Eli Rotenberg
Advanced Light Source

Jyoti Katoch
Carnegie Mellon University
MAESTRO and U

https://sites.google.com/a/lbl.gov/maestro/

ALS-U: Enhanced Brightness
MAESTRO-U: Optics upgrade to preserve brightness

25–30x signal improvement over today’s MAESTRO
Angle-resolved photoemission spectroscopy

\[(\theta, KE, \Phi_W) \rightarrow (k, \omega)\]
The ultimate spatial resolution

**too big**

macroscopic dimensions
100 nm

**too small**

atomic dimensions
~ 1 nm

**just right**

large enough for band structure, small enough to isolate quantum fluctuations and confined states
5-10 nm

We do this now:

bulk properties of small things.
(ongoing 10 years of transformative, pre-ALS-U science)

Like an STM: we would lose momentum resolution.

>> 10 years of new, transformative, ALS-U enabled science

(Bi,Mn)Te₃
Helical Dirac Fermions

(Bi,Mn)Te₃
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Helical Dirac Fermions
(Bi,Mn)Te₃

Large enough for band structure, small enough to isolate quantum fluctuations and confined states
5-10 nm

Yazdani NPhys 2011

Kapitulnik 2003

Yazdani Science 2010

BSCCO
High-Tc superconductor

(Ga,Mn)As
Anderson Localization

Kapitulnik 2003

Yazdani Science 2010

Yazdani NPhys 2011

Kapitulnik 2003

Yazdani Science 2010

WS₂ on graphene

SEM

nARPES

WS₂ on graphene

SEM

nARPES

WS₂ on graphene

SEM

nARPES

WS₂ on graphene

SEM

nARPES
Higher spatial resolution in nanoARPES

Higher spatial resolution nanoARPES provides opportunity to study the electronic band structure of novel 2D material with smaller grain size.

The electronic properties of vertical/lateral 2D heterostructures are affected by immediate surrounding as well as twist angle between the constituent 2D stacking layers.

nanoARPES with spatial resolution of 5-10 nm is a powerful technique to investigate the effects of nanoscale sized inhomogeneities in the surrounding environment that cause strong variations of electronic interactions in 2D based heterostructures.

2D based vertical/lateral heterostructures

Twistronics


Cao et al., nature (2018)
Simultaneous transport and spatially-resolved nanoARPES measurements.

Direct investigation of the conducting edge states, valley Hall effect, and exciton Hall effect in TMDCs.
New tender x-ray beamline

Chenhui Zhu
Advanced Light Source

Pupa Gilbert
Univ. of Wisconsin–Madison
Tender beamline layout

• 1–5 keV (up to 8 keV at 2nd branch), full length ID, linear polarization
• Branchline 1: grating mono (1–5 keV), ~5 micron focus
• Branchline 2: crystal mono (2–8 keV), ~100 nm focus
Tender XPCS: probe fast spontaneous fluctuations across broad length scales

Complex fluids
Noel Clark, Colorado

Metal organic framework
Omar Yaghi, Berkeley

Cell membrane
Sunil Sinha, UCSD

• Physics
• Biology
• Chemistry
• Energy
• Materials science
• Nanotechnology

In-situ environments:
Ambient pressure XPS, tensile, IR, printing...

Flexible electronics
Zhenan Bao, Stanford
Why tender-x-rays (2-8 keV)?
Because they can probe most of the periodic table (1s, 2p, 3d orbitals)

COherent Microscopy of Earth-samples with Tender-x-rays (COMET), if funded by NSF in 2019, COMET will lead the world in tender ptychography, and will be fully operational in 2022, well before ALS-U.

Pupa Gilbert, UW-Madison
we will finally access **bone nanocrystals** and **collagen fibrils** in 3D, in pristine bone

seen in their natural state, that is, interspersed nanocrystals and collagen fibrils, thus revealing the size, shape, and orientation of each nanocrystal and fibril, observing at once many nanocrystals and fibrils, their position and orientation, and how these change during mechanical stresses. Thus revealing the **functional** structure of bone
New soft x-ray beamline

Sujoy Roy
Advanced Light Source

Alex Frañó
UC San Diego
FLEXON: A high-brightness coherent soft X-ray beamline for probing roles of multiscale heterogeneity in quantum materials

FLuctuation and EXcitation of Orders in the Nanoscale

XPCS  nRIXS  nRSoXS
FLEXON is coming to Sector 10

Beamline Energy: 400–1400 eV
Full polarization control

- A unique facility with unique capabilities will lead to world-class discoveries in quantum materials.
- Evolution of nanoscale electronic and magnetic features across multiple scales in space and time.

Sample synthesis facility connected to endstations
Phase coexistence as a form of equilibrium

Different phases in equilibrium segregate into regions → govern the macroscopic behavior

Naturally occurring

Ice+water

Magnetic (electronic) domains

Human-assisted
Domain network designed by implanted ions

Phase coexistence at the nanoscale \rightarrow \text{FLEXON}

Challenge: interplay between superconductivity and charge order?

Solution: Apply electric currents, monitor evolution upon removing superconductivity

High current densities (critical currents) require small nano-scale devices...nano probes! \rightarrow need multimodal approach!

Phase coexistence at the nanoscale → FLEXON

**Challenge:** interplay between superconductivity and charge order?

**Solution:** Apply electric currents, monitor evolution upon removing superconductivity

High current densities (critical currents) require small nano-scale devices...nano probes!

→ need multimodal approach!

Apply high current densities across nanodevices:

1. **nRSXS**: Visualize phase separation: what happens at the boundary?, etc..
2. **nRIXS**: Visualize excitations at the nano boundaries: plasmon and charge excitations
3. **XPCS**: Detect temporal fluctuations and mesoscale coherence: pair-density wave, nonergodic behavior compared to regions without current
Questions

General ALS-U information: als.lbl.gov/als-u
Additional Slides
Stages of a DOE project and where ALS-U is

**INITIATION**
- Identify Mission-Related Need
  - CD-0 Approve Mission Need (Sept 27, 2016)

**DEFINITION**
- CD-1 Approve Cost Range (Sept 21, 2018)
  - Baseline (CD-2) is when the scope, cost, and schedule are fixed

**EXECUTION**
- CD-2 Approve Performance Baseline
- CD-3 Approve Start of Construction

**CLOSEOUT**
- CD-4 Project Completion

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- Currently working on preliminary design—leads to performance baseline
  - Baseline (CD-2) is when the scope, cost, and schedule are fixed
# Review committees

## Steering committee
(internal to LBNL):

- Steve Kevan
- Howard Padmore
- Zahid Hussain
- Kevin Wilson (CSD)
- Peter Fischer (MSD)
- Ken Chow
- Christoph Steier
- Ken Goldberg

## Ad hoc committee
(external to ALS):

- Lou Terminello (PNNL, SAC)
- David Prendergast (LBNL, SAC)
- Steve Hulbert (BNL, ESAC)
- Andy Broadbent (BNL, ESAC)
- Brandy Toner (Minnesota)
- Frances Houle (LBNL)
- Uwe Bergmann (SLAC)
- Tom Rabedeau (SLAC)
- Oleg Chubar (BNL)
Beamline working group

Andreas Scholl  Sujoy Roy
Will Chueh     Yi-De Chuang
Ashley White   Alexei Fedorov
Sue Bailey     Eli Rotenberg
Corie Ralston  Matthaeus Leitner
Martin Kunz    Simon Morton
Mike Martin    Jeff Takakuwa
Alex Hexemer   Chenhui Zhu
Hendrik Bluhm  Ethan Crumlin
Jinghua Guo    Aaron Bostwick
David Shapiro  Chris Jozwiak
Elke Arenholz  Padraic Shafer