Amplifying science insights - synergistic partnerships between EMSL and Light Sources

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Supplemental facility information
At EMSL, we focus on fundamental research to predict molecular and sub-atomic processes underpinning biological and environmental functions.

The Functional and Systems Biology Area focuses on elucidating and harnessing the biochemical pathways that connect gene functions to complex phenotypic responses through a deep understanding of interactions within cells, among cells in communities, and between cellular membrane surfaces and their environment for microbes, fungi, and plants. The following Integrated Research Platforms enable this science:

**Functional Omics**—We integrate transcriptomic, proteomic, and metabolomic analyses to uncover biological processes in plant, fungal, and microbial systems.

**Molecular Bioimaging**—We image the structure and location of proteins and other biomolecules at nanoscale spatial and temporal resolutions.

**Cellular Dynamics**—We uncover the molecular signals within and between cells as they respond to their environment and other organisms.

The Environmental Transformations and Interactions Area focuses on the mechanistic and predictive understanding of environmental, microbial, plant, and ecological processes in above and belowground ecosystems, the atmosphere, and their interfaces. The following Integrated Research Platforms enable this science:

**Biogeochemical Transformation**—We investigate how molecular interactions at the Earth’s land, water and air interfaces transform and transport nutrients and contaminants within the environment.

**Isotope and Chemical Analysis**—We track the fate of isotopes and analyze the chemistry of biological and environmental systems.

**Molecular Plant Phenotyping**—We probe the interaction between genes and the environment to understand, predict and control plant traits.
The Advanced Light Source (ALS) provides users from around the world access to the brightest beams of soft x-rays, together with hard x-rays and infrared, for scientific research and technology development in a wide range of disciplines including biological and environmental sciences.

**Micro X-Ray Absorption Spectroscopy Beamline 10.3.2**
Beamline 10.3.2 provides for the rapid collection of X-ray fluorescence maps and point X-ray absorption and powder diffraction data with ~1-5 μm spatial resolution.

*Coralie cryogenic spectromicroscopy uncovers selenium bioreduction products*
- Synchrotron hard X-ray microprobe (SNOM) setup. Crystallography reveals cryogenic features: evaporation, Fe and Ni microprobe measurements. (A) CLM77X stage (B) View of the nitrogen grid holder tongue installed on the mounting frame. (C) View of the stage at beamline 10.3.2 with the sample-transfer tongue inserted. The sample is oriented at 45° to the incident beam, and micro-XRF is performed in transmission mode.

**Scanning Transmission X-ray Microscopy (STXM) Beamlines 5.3.2.2/11.0.2**
Both beamlines provide for the rapid collection of 3D X-ray absorption data with submicron spatial resolution for quantitative volumetric investigations on chemistry and structure of diverse environmental samples.

*Airborne soil organic particles generated by precipitation*
- A schematic illustration of the raindrop mechanism.
- Airborne soil organic particles (ASOP) compositional maps with sp2 and non-sp2 carbon shown in red and green, respectively. C) Correlation between the total carbon absorption/area equivalent diameter ratio and sp2 carbon content.

After rain events, sub-micron solid particles, with a chemical composition consistent with soil organic matter, contributed up to 60% of atmospheric particles. Chemical imaging and micro-spectroscopy analysis of physicochemical properties suggest that these particles may have important impacts on cloud formation and efficiency of solar radiation. B. Wang et al., Nat. Geosci. 9, 435 (2016).

**Non-destructive Synchrotron Infrared Spectral Imaging**

\$\text{SFIIR}\$ Spectromicroscopy at BL 1.4 & BL 5.4
- Spatial/temporal distributions and chemistry of functional groups of molecules
- 2-15 μm focused beam spot & spatial resolution
- Seconds to minutes temporal resolution

\$\text{SFIIR}\$ spectromicroscopy images (200 μm by 150 μm) showing the co-localization of microbial biomolecules and minerals in a living microbe. (Insert) sampling locations. Valdesova et al. Front in Microbiology 9, 2018.

\$\text{SFIIR}\$ Nano Spectroscopy at BL 2.4 & BL 5.4
- Spatial distributions and chemistry of functional groups of molecules
- 2-30 nm focused beam spot

(a) A schematic of the synchrotron infrared nano-spectroscopy (SINS) setup that combines synchrotron IR with scattering nanofield Optical Microscope (SNOM). (b) SINS can be applied to hard and soft matter, including biomolecules, proteins, bacteria, fungi, and other biomaterials to identify and measure local surface chemistry. (Wu et al. Nature, 541, 2017)
Stanford Synchrotron Radiation Lightsource
http://www-ssrl.slac.stanford.edu

Contact: John Bargar; bargar@slac.stanford.edu

MicroXAS imaging
- Spatial distributions and chemistry of trace and major elements
- 2 μm focused beam spot
- Oxidation states and chemical forms of elements

<table>
<thead>
<tr>
<th>BL</th>
<th>2 μm resolution</th>
<th>Energy (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-3</td>
<td>5.0-24</td>
<td></td>
</tr>
<tr>
<td>10-2</td>
<td>5.0-24</td>
<td></td>
</tr>
<tr>
<td>14-3</td>
<td>2.1-5</td>
<td></td>
</tr>
</tbody>
</table>

Co-localized U and Zr in Chernobyl particles

Pyrite oxidation in shale exposed to fracture fluid

Small angle x-ray scattering (SAXS)
- Size distributions of nanoscale materials
- 3D details of macromolecules, nanoparticles, surfaces, pores.

<table>
<thead>
<tr>
<th>BL</th>
<th>Energy (keV)</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-5</td>
<td>4.6-16.0</td>
<td>SAXS</td>
</tr>
<tr>
<td>4-2</td>
<td>6.0-17.0</td>
<td>Bio-SAXS</td>
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Transmission X-ray microscopy (TXM)
- 2D Imaging & 3D nano-tomography
- Solids, soil-microbe aggregates, and rocks
- Energy specific imaging.

<table>
<thead>
<tr>
<th>BL</th>
<th>0.6 μm resolution</th>
<th>5-14 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6-2</td>
<td>30 nm resolution</td>
<td></td>
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Metals incorporation of a single catalyst particle

X-ray absorption spectroscopy (XAS)
- Electronic structure (oxidation states)
- Molecular structure
- Interfaces, aqueous solutions, biological materials, and amorphous materials.

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<thead>
<tr>
<th>BL</th>
<th>Energy (keV)</th>
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<tbody>
<tr>
<td>4-1</td>
<td>5.0 – 38</td>
</tr>
<tr>
<td>4-3</td>
<td>2.4 – 14</td>
</tr>
<tr>
<td>7-3</td>
<td>5.4 – 32 (bioXAS)</td>
</tr>
<tr>
<td>9-3</td>
<td>5.0 – 30 (bioXAS)</td>
</tr>
<tr>
<td>11-2</td>
<td>5.0 – 38</td>
</tr>
<tr>
<td>14-3</td>
<td>2.1 – 5 keV</td>
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X-ray powder diffraction (XRD)
- Identification of crystalline materials
- Coherent scattering domain size
- Unit cell dimensions

<table>
<thead>
<tr>
<th>BL</th>
<th>Energy (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-1</td>
<td>4-14.5 keV</td>
</tr>
<tr>
<td>11-3</td>
<td>12.7 keV (1.0 Å)</td>
</tr>
</tbody>
</table>

User proposal deadlines:
- X-ray techniques: May 1, Aug 1, Nov 1
- Microcrystallography: Jul 1, Dec 1, Apr 1

SSRL Structural Molecular Biology program supported by DOE BER and NIH National Institute of General Medical Sciences http://ssrl.slac.stanford.edu/smb/index.html
Advanced Photon Source

Over 20 beam lines devote some of their scientific effort to Hydrobiogeochemistry. All beamlines can receive actinide samples and sectors 10, 13, and 20 have nearby laboratory facilities. The Advanced Photon Source offers annual courses on synchrotron science open to everyone from students to senior scientists.

- **Sector 2**: sub-micron X-ray microscopy, ptychography, tomography
- **Sector 5**: X-ray powder diffraction (XRD), small angle x-ray scattering (SAXS), X-ray absorption spectroscopy (XAS)
- **Sector 9**: “tender” XAS, hard x-ray nanoprobe- 30 nm resolution (transmission, fluorescence, ptychography)
- **Sector 10**: (MRCAT/EnviroCAT): low-concentration XAS, fluorescence microscopy, spectromicroscopy
- **Sector 11**: Powder XRD
- **Sector 12**: XAS, SAXS
- **Sector 13**: GSECARS: X-ray absorption spectroscopy, X-ray tomography, microscopy, spectromicroscopy, XRD microscopy
- **Sector 18**: BIO-CAT: SAXS
- **Sector 20**: PNCCAT: X-ray absorption spectroscopy, X-ray Raman, fluorescence microscopy, spectromicroscopy
- **Sector 32**: Transmission x-ray microscopy, transmission nanotomography

Run Cycle | Run Dates | Proposal Submission Deadline
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2019-3 | Oct - Dec 2019 | July 5, 2019
2020-1 | Feb - Apr 2020 | Oct 25, 2019
2020-2 | June - Aug 2020 | Feb 28, 2020

X-ray fluorescence microscopy: 2D elemental mapping

X-ray absorption spectroscopy (XAS): Element specific local atomic structure

X-ray tomography: 3D elemental or pore structure imaging

Fully equipped geomicrobiology laboratories available to BER funded Argonne SFA collaborators within half mile of the synchrotron
National Synchrotron Light Source-II (NSLS-II)

NSLS-II is a state-of-the-art 3 GeV electron storage ring. The facility offers scientific and industrial researchers an array of beamlines with X-ray, ultraviolet, and infrared light to enable breakthroughs in critical areas such as energy security, chemistry and catalysis, biosystems, earth and environment.

- **3-ID**: Hard X-ray Nanoprobe (X-ray microscopy, ptychography, tomography)
- **4-BM**: X-ray Fluorescence Microprobe (micro-EXAFS, -XRD, -XRF, tomography)
- **5-ID**: Sub-micron Resolution X-ray microscopy
- **6-BM**: “Hard” X-ray absorption spectroscopy
- **7-BM**: Quick X-ray absorption spectroscopy
- **8-BM**: “Tender” X-ray absorption spectroscopy and imaging
- **8-ID**: Inner-shell spectroscopy
- **18-ID**: Transmission X-ray Microscopy
- **28-ID**: High-energy powder diffraction and pair distribution function analysis

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**Impacts of sea level rise on arsenic mobility in coastal soils**
- Global mean sea levels are expected to rise by 0.8 m by 2100
- Potential impacts to large populations and contaminated sites along coasts
- Investigate soil As speciation under two inundation scenarios: sea or river water as a function of Eh

**RESULTS**
- Arsenic conditions resulted in reduced As species (more for river water inundation)
- As release into solution was 250 times higher for river water than for sea water
- Iron in sea water (e.g., Fe(II)) stabilized As as solid phase and was inhibited by DBP (dissimilatory metal reducing bacteria); solid phase speciation in this soil was dominated by Fe-bearing As oxyhydroxides rather than sorption complexes
- River water did not exhibit reductive dissolution or dissimilatory Fe reduction

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**Plant uptake and trophic transfer of engineered nanomaterials (NM)**
- Agronomic application of NM (phytomass technology) has potential to alter conventional plant production systems
- Controlled release of agriculturals (e.g., fertilizers, pesticides and herbicides) and target-specific delivery of biocides (e.g., nucleotides, proteins and antibiotics)
- Investigate effect of surface charge on the uptake and translocation of NM in plants

**RESULTS**

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**Left**: CeO<sub>2</sub>-NM accumulation at rhizosphere and epidermis
**Middle**: Aquatic (between cells) transport of CeO<sub>2</sub> in root cortex
**Right**: Endocytosis may be mechanism of CeO<sub>2</sub> uptake into cells from root apoplasia

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**Contact**: Ryan Tappero; rtappero@bnl.gov

**Run Cycle**
- **Fall 2019**: Sep - Dec 2019, May 31, 2019
- **Spring 2020**: Jan - Apr 2020, Sep 30, 2019
- **Summer 2020**: May - Aug 2020, Jan 31, 2020

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To Become a NSLS-II User: www.bnl.gov/po/usrguide
Beam time is available at no charge to researchers and is granted through a peer-review proposal process.
Upcoming events and announcements
virtual meeting

National School on Neutron and X-ray Scattering
June 13 - 27, virtual meeting

Visit the website:
APS/IIT Summer XAFS School
July 12 - 17, virtual meeting

Visit the website:
aps.anl.gov/APS-Reminders/2020-07-12/apsiit-summer-xafs-school
August 25 - August 28, virtual meeting

als.lbl.gov/user-meeting/
SSRL EXAFS Summer School
Late August - Early September

Visit the website for updates:
ssrl.slac.stanford.edu/conferences/workshops/exafs
2018/index.html
SSRL/LCLS Annual Users’ Conference & Workshop
September 30 – October 2, virtual conference

Visit the website:
conf.slac.stanford.edu/ssrl-lcls-2020/
SSRL and ALS plan to host a session at AGU 2020 “Synchrotron Environmental Science-VIII”

JOIN US!

Visit the AGU website for updates: agu.org/Fall-Meeting
EMSL, ARM, and JGI plan to co-host the AGU 2020 session “Collaborate with a DOE User Facility: Learn About Available Expertise and Resources, Open Call Opportunities, and Important Tips for Submitting Successful Proposals”

JOIN US!

Visit the AGU website for updates: agu.org/Fall-Meeting
The deadline for this year’s summer school has passed but be on the lookout for next year’s opportunity. Postdoc and early career researchers are welcome to apply. More information about the 2021 Summer School will be available in December.

pnnl.cvent.com/2020SummerSchool