



## BRIGHT Beamlines Complement the Current Operational Beamlines at the Australian Synchrotron

The eight new BRIGHT Beamlines that are under construction at the Australian Synchrotron will strongly complement the existing operational beamlines at the facility. The full suite of 18 beamlines will operate from within six Beamline Groups: *Crystallography, Imaging, Diffraction, Scattering, Microscopy, and Spectroscopy*. The following document highlights the key capability differences between the beamlines within each beamline group.

### **Crystallography**

The *Crystallography Beamline Group* is formed by the three Macromolecular Crystallography Beamlines, MX1, MX2 and the new *High Performance Macromolecular Crystallography Beamline* (MX3). MX3 with the smallest and brightest X-ray beam will be used for extremely challenging macromolecular crystallography studies, and will build upon the successes and strongly complement our MX1 (bending magnet based) and MX2 (undulator-based, micro-focused) beamlines.

MX3 will be capable of providing a very high-flux, micro-focused X-ray beam for small and weakly diffracting protein crystals. The beamline will provide three modes of operation: goniometer, serial crystallography and in-tray screening. The beamline will be powered by a 3m in-vacuum undulator, and the proposed optical system will maximise flux at the sample position for a beam that is only several microns in size. In order to produce the required high X-ray flux, the beamline use a Double Multilayer Monochromator (DMM) instead of the normal silicon-based Double Crystal Monochromators (DCM) that are in operation on MX1 and MX2. This will increase the bandpass and brightness of the X-ray beam; however, this will mean that Multi-wavelength Anomalous Dispersion (MAD) experiments will not be feasible. The beamline will specialise in high flux, high speed data collection on micro crystals with a high degree of automation for crystal location and data collection.

| Beamline | Full beam size ( $\mu$ ) | Min collimated beam size ( $\mu$ ) | Full beam flux at sample (ph/s) | Key Capabilities & Science  |
|----------|--------------------------|------------------------------------|---------------------------------|---|
| MX1      | 180x150                  | 50x50                              | $3.4 \times 10^{11}$            | Very stable beam, Kappa-circle, Low energy X-rays available, Screening, MAD/SAD<br>Chemical & Protein Crystallography, Weak anomalous data, Medium sized crystals |

|                                 |       |      |                       |   |
|---------------------------------|-------|------|-----------------------|---|
| <b>MX2</b>                      | 22x12 | 10x8 | 2.40x10 <sup>12</sup> | Hot beam, Small crystals, High throughput, MAD/SAD studies<br>Weakly diffracting and small crystals.<br>Chemical & Protein Crystallography, Preferred beamline for pharmaceutical industry  |
| <b>MX3<br/>(proposed specs)</b> | 8x2   | 2x2  | >6x10 <sup>13</sup>   | Micro-focused, Very hot beam, Variable beam size suitable for micro crystals, serial crystallography and injector studies<br>Serial crystallography via goniometer, fixed targets and injectors. In-tray screening and collection |

### Imaging

The *Imaging Beamline Group* consists of the *Imaging and Medical Beamline (IMBL)* and the new *Micro-Computed Tomography (Micro-CT) Beamline*.

IMBL is a flagship beamline at the Australian Synchrotron; able to conduct Micro-beam Radiotherapy (MRT) studies, as well as video speed radiography and computed tomography studies. The long length of IMBL (~140m) allows the beam to expand in size so as to be able to provide a large field-of-view, and also enables propagation phase contrast imaging studies to be undertaken. IMBL’s superconducting multipole wiggler source generates a very high flux-X-ray beam with energies up to 300 keV. Both monochromatic and multi-wavelength pink beam modes are available; however the minimum spatial resolution of CT measurements on IMBL is of order 10 microns or larger. Robotic platforms facilitate CT studies of large objects (up to 1 m and 100 kg), as well as facilitating *in vivo* imaging studies. Human imaging studies will also be possible from 2021 onwards.

The *Micro-CT* beamline will use X-rays from a bending magnet source and will be optimised for high-throughput CT studies of small objects, with sub-micron spatial resolution down to 0.2 microns (using Fresnel-zone-plate optics - the *nano-CT* set-up). Standard micro-CT measurements are expected to take place with spatial resolutions down to 0.7 microns, and will also encompass in-line phase contrast measurements. Other novel (grating- and speckle-based) phase contrast measurements will also be possible on Micro-CT, although with poorer spatial resolution (down to 4 microns). Depending on the speed of measurement or the desired spatial resolution, monochromatic, filtered white-beam, or filtered pink-beam X-ray CT measurements will be possible. A range of different measurement modalities will be possible, including “on-the-fly” scanning, “step-&-shoot” scans, helical scans, laminography and tomosynthesis CT modes. A table-mounted 6-axis sample-exchange system (robot) will provide a high-throughput capability for small samples (up to 100 samples per magazine; max width 13 mm; max height 100 mm - samples larger than the beam field-of-view can in general be imaged via image stitching procedures and, for tall samples, using helical scans).

| Beamline    | Full beam size (mm) | Min voxel size (µm) | Energy Range (keV)    | Key Capabilities & Science   |
|-------------|---------------------|---------------------|-----------------------|--|
| <b>IMBL</b> | 300 (h) x30 (v)     | 10                  | SCMW<br><br>Up to 300 | Monochromatic and filtered white and pink X-ray beams<br>In vivo studies, Large sample CT<br>Broadbeam and Microbeam Radiotherapy,<br>Propagation phase contrast imaging and computed tomography<br>Pre-clinical low-dose imaging and CT |

|          |                 |     |                       |  |
|----------|-----------------|-----|-----------------------|--|
| Micro-CT | 64 (h) x 10 (v) | 0.2 | Bend Magnet<br>8 – 40 | Monochromatic and filtered white and pink X-ray beams<br>CT modes: “on-the-fly”, “step-&-shoot”, helical, laminography and tomosynthesis<br>Propagation-, grating- and speckle-based phase contrast modalities |
|----------|-----------------|-----|-----------------------|--|

### Diffraction

The *Diffraction Beamline Group* when formed will consist of the current *Powder Diffraction beamline (PD)*, and the newly constructed *Advanced Diffraction and Scattering Beamlines (ADS-1 and ADS-2)*.

The *Powder Diffraction* beamline uses a bending magnet source to undertake rapid and sensitive atomic scale structural studies via powder X-ray diffraction (XRD). The majority of measurements using the PD beamline are *in situ* or *in operando* studies of chemical or physical processes (eg nucleation, crystallisation, or corrosion), or studies of functional and energy materials while under operating conditions (eg batteries, catalysts, molecular sieves, or gas storage frameworks). The majority of PD studies makes use of a *Mythen II* microstrip detector, allowing diffraction profiles to be collected in as little as a few seconds. The PD beamline has a large number of sample environments, capable of housing samples under extremes of temperature (10 – 1870 K), pressure (up to ~10 GPa), or under gas or fluid flow. High sample throughput capabilities are available including a sample changing robot and capillary auto-alignment system.

The *Advanced Diffraction and Scattering* beamlines (ADS-1 and ADS-2) will be optimised for a range of leading-edge diffraction and scattering measurements. ADS-1 and ADS-2 will be able to operate simultaneously with multiple sample configurations and sample environments using high-energy monochromatic and polychromatic X-rays that will be generated using a powerful Superconducting Multipole Wiggler (SCMW) source. The optics layout will maximise the flux at the sample position and provide versatility in possible beam sizes. Both beamlines will have state-of-the-art hybrid pixel detectors with CdTe sensors for maximum detection efficiency and sensitivity for monochromatic diffraction experiments. In addition to powder X-ray Diffraction, ADS-1 will also be capable of undertaking single crystal diffraction studies (complementing MX1, MX2 and MX3), energy-dispersive diffraction for strain scanning and probing of bulk material, as well as a range of imaging and computed tomography studies (complementing IMBL and Micro-CT). ADS-1 and ADS-2 will enable the study of many scientific applications including:

- Studies of mineral formation and recovery under extreme conditions of temperature and pressure;
- Non-destructive detection of corrosion, cracking, fractures, textures, strains and deformations in large manufactured objects across the energy, automotive, transport, defence and aerospace sectors;
- Maintenance and component failure studies of engineering infrastructure;
- Studies of glasses and amorphous alloys;
- Characterisation and optimisation of energy storage, production and conversion systems e.g. batteries, fuel cells and thermoelectric materials.

| Beamline | Beam Dimensions (h x v) | Energy Range (keV) | Key Capabilities & Science |
|----------|-------------------------|--------------------|----------------------------|
|----------|-------------------------|--------------------|----------------------------|

|        |  |                              |  |
|--------|--|------------------------------|--|
| PD     | 3 x 1 mm <sup>2</sup>                                  | Bending Magnet<br>8 – 21     | Capillary, and flat plate samples<br>Hot air blowers (max 950 °C), furnaces (max 1700 °C), Liq. N <sub>2</sub> cryostream (80 – 480 K), cryostat (10-300 K), gas and liquid flow cells.<br>Multiple battery carousel; Diamond Anvil Cell (max 10 GPa).<br>Mythen II microstrip detector, Mar 345 2D detector<br><b>Robotic sample changer and capillary auto-alignment system</b>  |
| ADS -1 | 20 x 5 μm <sup>2</sup><br>-<br>10 x 10 mm <sup>2</sup> | SCMW<br>50 – 150             | White; pink; and monochromatic X-rays<br>Samples: powders, compacts, metals, alloys and assemblies; small and large size (up to 800 mm) with maximum mass of up to 300 kg.<br>Sample environments: gas, uniaxial and multi-anvil pressure cells; temperature (heaters, furnaces and cryostream) combined with gas flow and other cells; and User-supplied stages/environments.<br>White beam experiments: Energy dispersive diffraction; High resolution 3D strain scanning; Laue diffraction<br>Monochromatic beam experiments: In situ powder diffraction, Single crystal measurements including diffuse scattering and techniques such as High pressure cells; Rapid texture analysis and 2D materials mapping<br>Imaging and Computed Tomography |
| ADS-2  | 4 x 0.5 mm <sup>2</sup>                                | SCMW<br>45.3, 74.0 &<br>86.8 | Monochromatic X-ray diffraction; Three fixed monochromatic wavelengths<br>Samples up to 50 kg.<br>Powder diffraction, single crystal diffraction, high throughput applications.<br>Total Scattering or Pair Distribution Function (PDF) analysis (high momentum transfer, Q <sub>max</sub> > 30 Å <sup>-1</sup> )  |

## Scattering

The *Scattering Beamline Group* will consist of the *Small and Wide Angle X-ray Scattering Beamline* (SAXS/WAXS), and the new *Biological Small Angle X-ray Scattering Beamline* (BioSAXS).

The *Small and Wide Angle X-ray Scattering beamline* uses a high brilliance in-vacuum undulator source to generate a high flux monochromatic X-ray beam for the study of a range of nanoscale structures and materials. This beamline is ideally suited to the study of polymeric materials, organic solar cells and electronics, advanced drug delivery systems, surfactants and liquid crystal systems, food and agricultural products, nanomaterials, and protein structures and complexes. The SAXS/WAXS beamline has the capability of studying a wide variety of samples: from proteins in solution with in-line size exclusion chromatography and the CoFlow set-up to minimise radiation damage; other solution scattering studies; solid samples in transmission; or thin films in glancing incidence mode. Due to having a Si-based monochromator the beamline can also conduct Anomalous Small Angle X-ray Scattering (ASAXS) measurements using by scanning a range of different photon energies.

The *Biological Small Angle X-ray Scattering* beamline will combine a superconducting undulator with a double multilayer monochromator to produce a very high brilliance X-ray beam. The BioSAXS beamline will support solution scattering from nanoscale chemical and biological systems using in-line size exclusion chromatography and the new CoFlow autoloader system. Complex sample environments can be accommodated to enable rheometry, microfluidics, temperature and pressure control, and automated high-throughput studies of liquid phase systems. A high speed in-vacuum detector will enable low noise data to

be acquired over a wide Q-range and provide millisecond time resolution for the study of changes in protein structure, protein-protein interactions, and enzymatic reactions.

| Beamline         | Beam size ( $\mu\text{m}$ )  | Energy Range (keV)   | Key Capabilities & Science  |
|------------------|--|--|---|
| <b>SAXS/WAXS</b> | Focused:<br>250 (h) x 25 (v)<br><br>Defocused:<br>1000 (h) x 450 (v) | In-vacuum Undulator<br><br>5.5 - 21<br><br>Optimised for 8- 12 | Maximum flux: $8 \times 10^{12}$ at 12 keV<br>Q-range: SAXS - $0.0015 - 3.0 \text{ \AA}^{-1}$ ; WAXS - $0.6 - 10 \text{ \AA}^{-1}$<br><br>Solution scattering; SEC-CoFlow; Rheometry; Solid samples; GISAXS and GIWAXS for thin-film samples. Tensile stage; High temperatures ( RT - 600 °C)   |
| <b>BioSAXS</b>   | Focused:<br>300 (h) x 30 (v)<br><br>Defocused:<br>300 (h) x 400 (v)  | Superconducting Undulator<br><br>8-15                          | Maximum flux: $>10^{14}$ at 12 keV<br>Q-range: SAXS - $0.0013-4 \text{ \AA}^{-1}$<br><br>Solution scattering; Automated SEC-CoFlow; Microfluidics; Rheology experiments with Rheo-SAXS;<br><br>Linkam capillary cell for temperature variation studies; Sonochemistry using focused ultrasound; Studies of ferrofluids & magnetic nanoparticles |

## Microscopy

The *Microscopy Beamline Group* consists of the *Infrared Microspectroscopy Beamline (IRM)*, the *X-ray Fluorescence Microscopy Beamline (XFM)*, and the new *X-ray Fluorescence Nanoprobe*.

The *Infrared Microspectroscopy beamline* uses the high brilliance and collimation of the synchrotron light to generate diffraction limited chemical or biochemical infrared maps with a spatial resolutions of up to a few microns. This beamline is ideally suited to the analysis of microscopic samples e.g. small particles, thin films and layers within complex matrices, as well as single cells and complex biological systems. Infrared microspectroscopy is a non-destructive method that gives chemical and structural information for a diverse range of samples - biological and biomedical materials, forensic studies and food sciences, as well as cultural heritage and geological studies. Spatially resolved "heat maps" reveal the distribution of specific chemical functionalities within samples. Samples can be measured via a range of FTIR methodologies: transmission, reflectance, grazing incidence, or macro Attenuated Total Reflectance - a technique that is ideal for high-resolution studies of delicate biomaterials or other soft matter systems.

The *X-ray Fluorescence Microscopy (XFM) beamline* generates highly sensitive (better than parts-per-million) elemental maps for elements between Si and Se, as well as many heavier elements (Cd to Pu). The *XFM Milliprobe* configuration enables large areas to be mapped – up to  $0.6 \times 1.2 \text{ m}^2$  with 100 micron spatial resolution; while the *XFM Microprobe* enables mapping of  $140 \times 100 \text{ mm}^2$  as well as 3D elemental tomography with resolutions down to 1 micron. XANES spectroscopy enables characterisation of the chemistry and oxidation state of various elements within the sample. Simultaneous measurement of ultrastructure at 50 nm resolution via ptychography (Scanning X-ray Diffraction Microscopy) is available using the Microprobe.

The new *X-ray Fluorescence Nanoprobe* beamline will deliver more than an order of magnitude better resolution than the XFM beamline with comparable sensitivity. Elemental mapping down to ~60 nm resolution will be possible for most elements heavier than silicon. XANES spectroscopy will be available for substantial portions of the periodic table, including the important elements from Cr to Sr. Simultaneous ptychography will provide access to ultrastructure at around 15-nm resolution. Fluorescence tomography will be feasible, and cryogenic protection of radiation damage to biological specimens will enable effective elemental mapping at 100 nm resolution. Additional microscopy modalities will also be possible such as Scanning Transmission Microscopy and Differential Phase Contrast Microscopy. Other nanoscale and atomic scale characterisation measurements will be possible via Scanning Nano-Small Angle X-ray Scattering (nano-SAXS) and Scanning nano-diffraction.

| Beamline  | Min Resolution                                | Energy Range (keV)                                 | Key Capabilities & Science   |
|-----------|---|--|--|
| IRM       | 3-8 $\mu\text{m}$                             | Medium- to Far-IR (3800-550 $\text{cm}^{-1}$ )     | High speed Focal Plane Array (FPA) detector (64x64 pixels), or high sensitivity Mercury Cadmium Telluride (MCT) detector<br>Transmission, reflectance, grazing incidence, and macro-ATR modes.<br>Live cell studies, sample heating and cooling  |
| XFM       | 100 $\mu\text{m}$<br>1-2 (0.05) $\mu\text{m}$ | In Vacuum Undulator<br>4.1 - 27                    | Milliprobe: XRF maps and XANES Spectroscopy, Large area scanning of industrial and cultural heritage artefacts<br>Microprobe: XRF maps and XANES Spectroscopy, Ultrastructure measurement using ptychography (SXDM), elemental tomography<br>Cryogenic protection against radiation damage |
| Nanoprobe | 60 nm<br>15 nm                                | Cryo-cooled Permanent Magnet Undulator<br>2.2 – 15 | Elemental mapping & XANES down to 60 nm resolution, depending on concentration<br>3D elemental tomography<br>Cryogenic protection against radiation damage<br>Ptychography (SXDM) measurements gives ultrastructure at 15 nm.<br>Scanning nano-SAXS and nano-Diffraction                   |

### **Spectroscopy**

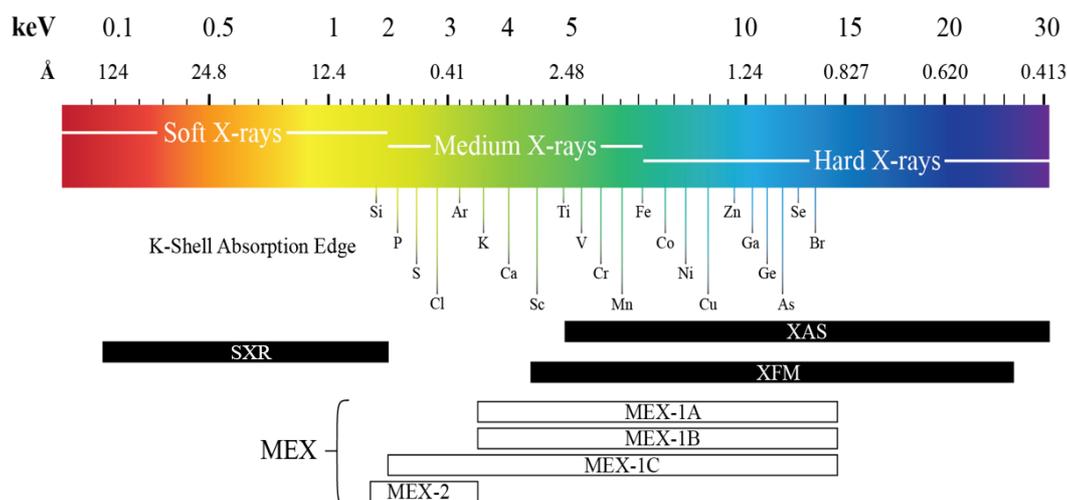
The *Spectroscopy Beamline Group* consists of 5 beamlines: the *Soft X-ray Spectroscopy* Beamline (SXR), the *Terahertz/Far-Infrared* Beamline (THz/Far-IR), the *X-ray Absorption Spectroscopy* Beamline (XAS), and the two new *Medium Energy X-ray Absorption Spectroscopy* Beamlines (MEX-1 and MEX-2). Together the beamlines of the Spectroscopy Group bridges a vast range of elements, functional materials and sample types.

The *Terahertz/Far-Infrared* beamline is the lowest photon energy beamline at the Australian Synchrotron. Far-Infrared radiation from a bending magnet source is used to undertake high energy resolution vibrational spectroscopy studies of gas-phase molecules, including reactions that take place in our upper atmosphere, as well as those that may take place in the atmosphere of other bodies in our solar system. Terahertz spectroscopy studies are also possible to characterise a wide range of condensed phase samples including batteries and new energy materials, composites, cultural heritage artefacts, forensic samples, cellular and other biological materials.

The *Soft X-ray Spectroscopy* beamline uses our lowest energy X-rays (90 – 2500 eV) from an Apple II variable polarisation undulator and operates in four different endstations on one of two soft X-ray branchlines. Soft X-ray spectroscopy studies typically examine the uppermost atomic layers of surfaces or thin-films, and require samples to be held under high vacuum or ultra-high vacuum conditions. The Soft X-ray main (Prevac) endstation is configured to undertake X-ray Absorption Spectroscopy (NEXAFS) and X-ray Photoelectron Spectroscopy (XPS) studies of low atomic number elements. This chamber can be replaced by a new *Toroidal Analyser* system to conduct Angle-Resolved Photoelectron Spectroscopy (ARPES) studies. These techniques are widely used to examine the atomic and electronic structures of catalysts, materials for flexible polymeric displays or next generation electronics, mineralogical surfaces, or environmental samples. The second branchline hosts the fast NEXAFS endstation for automated high-throughput X-ray Absorption Spectroscopy studies. Further downstream the Soft X-ray Imaging endstation enables structural studies of nanoscale structures using Coherent Diffraction Imaging (CDI) or soft X-ray ptychography.

The *X-ray Absorption Spectroscopy* beamline uses a wiggler source to deliver a very high brilliance X-ray beam over a wide range of energies (5 - 31 keV) in order to study the local bonding arrangements, chemistry and speciation (oxidation state) of elements including and heavier than scandium (1<sup>st</sup> row transition metals and above, up to uranium). Samples can be housed in complex environments (functional batteries, electrochemical cells, chemical reactors, or high pressure presses) for in situ studies, or in a low temperature cryostat to inhibit radiation damage of susceptible materials during measurement. XAS studies using this beamline are highly sensitive, able to characterise local structures and chemistry down to parts-per-billion sensitivity.

The new *Medium Energy X-ray Absorption Spectroscopy* (MEX) Beamlines (MEX-1 and MEX-2) will offer X-ray absorption spectroscopy capabilities that allow the study of the chemistry, speciation (oxidation state), and distribution of elements within materials. Unlike the current XAS and XFM beamlines that use wiggler and undulator sources that cater for measurements of the heavier metallic elements, the MEX beamlines are able to target the lighter elements (silicon, phosphorus, sulfur, chlorine, potassium, and calcium), as well as transition metal elements. The MEX beamlines use a bending magnet source (1.7 – 13.6 keV) and have been designed to offer enhanced capabilities for research in a diverse range of areas including health and human biology, agriculture and food science, environmental science, plant physiology and nutrition, material characterisation and advanced catalysts, geology and earth sciences, as well as museum and cultural heritage studies. The MEX-1 and MEX-2 beamlines will minimise radiation damage by using relatively large beam sizes (up to several mm<sup>2</sup>) and substantially lower flux densities than XAS. MEX-2 is the low energy beamline (1.7 – 3.5 keV), able to study elements between Si and K under vacuum conditions or a helium atmosphere. MEX-1 will give access to higher energy X-rays to study elements over the range S to Br. MEX-1 will operate a range of different endstations to enable X-ray Absorption Spectroscopy (XANES and EXAFS) of bulk specimens; studies using non-ambient sample environments; high energy resolution XAS studies; and micro-spectroscopy elemental mapping with a spot size between 2 and 10 microns.



The energy range and elemental coverage of the Medium Energy XAS beamlines

| Beamline      | Energy Range                                   | Key Capabilities & Science  |
|---------------|--|---|
| THz / Far-IR  | THz to Visible<br>(3800-550 cm <sup>-1</sup> ) | <p><i>Gas Phase studies:</i> Michelson interferometer; gas cells for reactive and non-reactive species; furnace studies; cooling to Liquid He temperatures</p> <p><i>Condensed Phase studies:</i> liquid cells, pressed discs in transmission; Attenuated Total Reflectance (ATR) measurements of surfaces or thin films.</p>   |
| SXR           | Apple II Undulator<br>100 - 3000 eV            | <p><i>Prevac Endstation:</i> XPS and NEXAFS. UHV (~10<sup>-10</sup> mbar) Sample cooling (to ~130 K); Flood gun; Sample preparation chamber - Low Energy Electron Diffraction (LEED), gas handling system, 4 point probe, Kelvin probe.</p> <p><i>ARPES Toroidal Analyser:</i> (UHV) Offline measurements using a high intensity vacuum ultraviolet lamp. Scanning tunnelling microscope (STM); 2D delay line detector; Dedicated sample growth chamber; Cooling to cryogenic temperatures.</p> <p><i>Fast NEXAFS Endstation:</i> HV (~10<sup>-7</sup> mbar) Easy sample loading; Flood gun; highly automated batch scanning.</p> |
| XAS           | 1.9 T Wiggler<br>5 - 31 keV<br>7 - 31 keV      | <p><i>Hutch B:</i> Transmission and fluorescence XAS; 10K cryostat; Capillary heating; Room temperature sample stage; 100 element Ge fluorescence detector.</p> <p><i>Hutch C:</i> In situ studies; Hydrothermal chemical reactions; D-DIA high pressure/high temperature press; 36 element Ge fluorescence detector.</p>   |
| MEX-1 & MEX-2 | Bending Magnet<br>MEX-1:<br>(3.5 - 13.6 keV)   | <p><i>MEX-1:</i> EXAFS and XANES in transmission and fluorescence. Sample in helium gas environment at ambient or variable temperatures (10-300K).</p> <ul style="list-style-type: none"> <li>- High Energy resolution EXAFS and XANES via a 5-crystal Johann-type spectrometer; 10 - 300 K; helium gas or vacuum.</li> <li>- Non-ambient sample environments: electrochemical cell, flow cell,</li> </ul>  |

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|--|---------------------------|--|
|  | MEX-2:<br>(1.7 – 3.5 keV) | pressure cell or furnace.<br>- Scanning X-ray fluorescence microprobe (2 - 10 $\mu\text{m}$ spot size).<br>Sample in helium gas atmosphere, variable temperature (80 – 500 K).<br><br>MEX-2:<br>- Bulk EXAFS and XANES in transmission, drain current and fluorescence.<br>- Bulk High Energy resolution-EXAFS and XANES via single crystal, dispersive refocusing Rowland circle-type spectrometer. |
|--|---------------------------|--|