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Introduction:

This report is an outgrowth of the NSLS-II Earth and Environmental Sciences Strategic Planning Workshop held at Brookhaven National Laboratory on January 22-23, 2008. Fifty two scientists registered for the workshop aimed at identifying key scientific drivers and beamline resources required by the scientific community at NSLS-II. This workshop also served to form the initial suite of Beamline Advisory Teams (BAT's) that wish to initiate Letters of Interest (LOI) for science focused beamlines at NSLS-II. This report builds upon an initial community report issued in July, 2007 (http://www.bnl.gov/x26a/download/NSLS2_MESGeo.pdf), and which contains additional recommendations not included here. We have structured this report to summarize 1) what some of the key scientific drivers for synchrotron based Earth and environmental research are likely to be; 2) an evaluation of community growth and likely utilization of NSLS-II resources; 3) recommendations for community needs at NSLS-II with regards to beamlines and infrastructure; and 4) community recommendations on how such resources are best advanced, for example as transitioned beamlines from the NSLS or as completely new NSLS-II beamlines. Also within this section we provide an overview of project BAT's the community is directly involved in and additional BAT's the community plans to lead in first round LOI efforts. At this point in time these include the following (along with the BAT spokespersons):

1. DWXAS - Damping Wiggler XAS Project Beamline (Bruce Ravel, NIST)
2. HXN – Hard X-Ray Nanoprobe Project Beamline (K. Evans-Lutterodt, BNL, interim)
3. PING - Powder Instrument Next Generation Project Beamline (John Parise, Stony Brook U.)
4. HiPHEX - High Pressure High Energy X-ray Beamline (Don Weidner, Stony Brook U.)
5. NICEST - Nanoscale Imaging of Chemistry and Electromagnetics with Soft x-rays (Chris Jacobsen, Stony Brook U.)
6. SREEL - Sub-micrometer Research in the Earth, Environmental, and Life Sciences (Antonio Lanzirotti, U. Chicago)

Specific community technical requirements for NSLS-II microprobe, EXAFS, scattering, STXM, and high pressure/high energy beamlines were also discussed. We summarize the beamline recommendations in tabulated form at the end of this report with estimates of anticipated beamline usage by the Earth and Environmental Sciences community.

Key Scientific Drivers for the Earth and Environmental Sciences Community:

The complexity of natural systems makes it unlikely that any single characterization method can provide all the information required about chemical speciation, spatial distribution, and physical associations needed to understand geological and environmental processes and model them. Thus, unlike many other communities utilizing synchrotron facilities, Earth and environmental science researchers frequent a variety of specialized beamlines and favor multi- and inter-disciplinary approaches to beamline operation. Thus characterizing the full breadth of resources required at NSLS-II by the community is difficult in a short white paper report. Synchrotron methods of particular interest to the community include x-ray absorption fine structure spectroscopy, x-ray microprobe, spectromicroscopy, microtomography, x-ray scattering, x-ray standing wave, infrared spectroscopy, and high-pressure experiments utilizing these techniques to examine minerals at deep earth conditions.

The source characteristics of NSLS-II will allow this community to extend such studies to unprecedented scales, furthering insights into geologically and environmentally relevant molecular scale processes. Environmental science in particular frequently involves the study of chemical speciation in natural materials that are heterogeneous down to the nanoscale. Some examples of the future scientific directions that NSLS-II will enable include the following:

1. *Mineral interfacial reactions at the sub-grain scale.* Nanometer scale spatial resolutions that will be enabled by NSLS-II will enhance our ability to evaluate the reactivity, bioavailability, and toxicity of environmental particulates and species adsorbed onto particulate surfaces. Such studies applied to airborne particulates will have atmospheric implications for climate forcing models. For example what is the tendency for particulate types to be cloud condensation nuclii; are given groups of particles hydophobic or hydroscopic; how do their surface chemistries control aggregation and transport? Similarly, studies of colloids and internal particle structures in natural systems are amenable to high resolution microspectroscopic analysis. Fundamental questions exist about whether such colloidal environmental particles form specific sizes of crystallites or

aggregates. It's clear these will require study at the nanometer scale. Questions also exist about what controls the surface area of materials in surface and subsurface settings. This work will also extend to studies of colloids in marine settings and their impact on carbon cycling in the oceans. Such studies will have significant implications in modeling transport and partitioning of environmentally and energy relevant species through sediments, soils, and rock and on climate change model development.

2. _Biogeochemical processes at the nanometer scale_. There is a fundamental need to assess the micro- and nano-scale heterogeneity of metals and metalloids in biogeochemical cycles. NSLS-II will allow for complementary soft and hard x-ray imaging techniques that will let us investigate at the cellular level how organisms interact with contaminants in natural environments. For example, fundamental questions exist about the toxicity and biogeochemistry of manufactured and natural nanoparticles in the environment. Such studies will allow us to better define electron transfer mechanisms between microbes and minerals and image cell wall contaminant chemistry. Also of great importance is an improved understanding of the binding mechanisms of natural organic matter and bacteria. Such studies will also enable new scientific disciplines such as "environmental genomics". The opportunities to examine how genetic variations in organisms affect their interactions with contaminant and nutrient metal species in the environment is driven by the rapidly increasing amount of nucleotide sequence data that is becoming available. Such studies remain in their infancy, but synchrotron based x-ray techniques are extremely well suited to help evaluate how specific genes influence the uptake of metals in plants and animals and for imaging these interactions at the cellular level.

3. _Fluid flow and contaminant transport at the pore scale_. In modeling contaminant transport, there is a vital need to evaluate how grain boundary geometries in natural systems influence the transport of chemical species in the subsurface. For example, perturbations on chemical migration may be much greater in fluids located in tight grain boundaries or within single mineral grains compared to fluids flowing through open cracks. Similarly, nanoscale confinement will alter the physiochemical properties of complex fluids and highly localized fluctuations in chemical conditions may occur due to leaching of mineral surfaces, nucleation and growth of new solids, and introduction of exotic elements from repositories (DOE, 2007). Advances in chemical imaging that will be made available by NSLS-II will offer excellent opportunities for imaging mineral-solution reactions in confined spaces *in-situ* within dense geologic media. Direct observations of pore scale transport may be possible, particularly in 3-dimensions using spatially resolved tomographic techniques. Since the average porosity of many subsurface lithologies has a natural size distribution at about 1 micron, the improvements in spatial resolution of x-ray micro- and nano- probes and for tomographic instruments will allow us to image and quantify the distribution of pore spaces, evaluate microbial distribution on pore walls, and micro-spectroscopically evaluate colloidal chemistry at mineral interfaces.

4. _In-situ and real time bulk x-ray diffraction of environmental materials_. In the 20th century, tools associated with room pressure and temperature (PT) bulk scattering techniques, coherent elastic and inelastic scattering from single crystals and powders for example, revolutionized our knowledge of the atomic arrangements and correlated vibrations in crystalline rock forming minerals. These static structure determinations, mostly based on the interpretation of the sharp Bragg diffraction from crystalline materials at room PT, provide the database of mineral structures often used as the starting point for the interpretation of spectroscopic data. Synchrotron X-rays allow us to push the boundaries of static studies to smaller samples for structure determination (µ-crystallography) and phase identification (µ-diffraction). As users push to ever greater resolution using XRF techniques, there will be an ever increasing need to correlate chemistry with phase (crystal structure). The high flux and brightness that will be available for scattering experiments at NSLS-II over a wide range of energies and employing optimized optics, detectors and sample environment allows us to conceive of experiments that open up whole new areas of research. These include real-time scattering to follow phase evolution as a function of time and environmental conditions (P, T, Eh, pH, fO_2 etc.). These techniques will allow us to mimic the conditions under which naturally occurring and engineered materials operate, and will provide

results that allow us to compare engineered samples and environments with those found in nature.

5. *Crystallographically challenged environmental materials*: Determination of the atomic arrangements (speciation) in liquids and in other poorly crystalline (nano)materials is often considered to be the domain of X-ray absorption, since in these materials long-range periodicity is less important and the interatomic arrangement is dominated by short-range interactions. Studies of the total X-ray scattering (Bragg + diffuse component) provides correlations beyond, say, the second or third shell provided by XAS and it is these distances that are crucial to interpretation of the over-all atomic arrangement. In principle all atomic pair correlations out to the limit of structural coherence, nominally restricted by the cluster or particle size, are available by Fourier transforming the elastic total scattering to produce the Pair Distribution Function (PDF). The two techniques, XAS and PDF, are naturally complementary: XAS provides element specificity at environmentally realistic concentrations while the PDF is a rich data-set of interatomic distances that allows a more unambiguous derivation of atomic arrangement. Key to the continued development of the PDF technique for environmental investigation is the provision of bright high energy ($E > 70$ keV) X-ray sources, and excellent signal-to-noise discrimination over a wide dynamic range, since the diffuse elastic scattering is some 10^6 times weaker than typical Bragg scattering. High energies are capable of penetrating sample cells and provide data to high angle (Q), which is necessary to properly normalize the elastic component of the total scattering that will be Fourier transformed to obtain PDF. Beyond the range of structural coherence it is important to follow processes such as incipient precipitation, nano-particle nucleation, ripening and shape change as a function of processing under different environmental conditions. While wide-angle X-ray scattering (WAXS), say above $Q=2$ Å^{-1}, provides information about interatomic distances, modeling the small angle X-ray scattering (SAXS) provides information on particle size and morphology. Both SAXS/WAXS measurements should ideally be performed simultaneously on the same sample contained in a controlled environment, in real time. While beamlines capable of such measurements are available none are optimized for the samples and sample environments likely to be of interest to the environmental scientist. Just as importantly, the researchers versed in these techniques are not environmental scientists and training opportunities for junior researchers in these areas are limited.

6. *Real-world x-ray absorption spectroscopy of environmental materials*: Bulk XAFS is -- and will remain -- a cornerstone of MES/LTG research. No other technique provides such versatile, non-destructive, element-specific access to local physical, chemical and electronic structure in complex matrices, in crystalline or noncrystalline materials, and *in-situ* under controlled environmental conditions. However, significant progress is still required in extending the capabilities of XAFS to allow for high resolution spectroscopy at real-world concentrations, abundances that are often below detection limits for current bulk XAFS techniques. A good example of this is mercury, which is a global environmental concern (and critical problem at some DOE sites). It is harmful in even low concentrations, accumulates in the food chain, and is governed by very complex and poorly-understood global atmospheric/terrestrial/marine cycling and molecular-scale transformation processes. The ability to study local speciation at realistic concentrations will greatly improve our understanding of these processes. The high flux and brightness of NSLS-II sources will provide unprecedented concentration sensitivity. XAFS studies of environmental samples also require analysis on various length scales, often in heterogeneous systems. The spatial resolution of XAFS measurements needs to be appropriate to the scale of the process being studied, and can vary from cm to mm, tens of microns (grain-scale), micron (cellular-scale), and nm (subcellular- and nanoparticle-scale). NSLS-II beamline will also be fundamental in advancing the possibilities for "mapping" spectroscopy? There is phenomenal potential utilizing XAFS research techniques in the mapping of speciation within biological and geological structures and its advantages in getting away from the "signal averaging" that you get in bulk XAFS. Thus a range of facilities (bulk, microprobe, nanoprobe) and versatility of focus are needed. NSLS-II will enable routine high-quality XAFS measurements over this wide range of spatial resolutions.

7. *Scientific Challenges in High-Pressure Research:* The scientific challenges in high-pressure research are manifold and involve overlapping scientific disciplines. In the past decade, advances in synchrotron x-ray based analytical techniques fostered remarkable breakthroughs in high pressure Earth sciences, including discovery of the post-perovskite phase of $MgSiO_3$ stable at more than 100 GPa, the unusually low melting temperatures of sodium, reaching 300 K at 118 GPa, complex structures of alkali metals at high pressure, observation of a spin state transition in iron under conditions in Earth's lower mantle, the changes in the bond characteristic of compressed graphite, and the measurement of the spin and charge order in chromium at high pressure. There are a number of current and future scientific challenges defined by the high-pressure Earth sciences community that will be able to be addressed using the unique capabilities that the NSLS-II facility will enable. The determination of the efficiency of the recycling of volatiles in the mantle and the identification of possible mineral reservoirs for volatiles at Earth's mantle are questions that at extreme conditions can only be studied in-situ utilizing synchrotron IR spectroscopy. Utilizing high pressure devices on wiggler based beamlines we will be able to make measurements of the melting temperature, elastic properties and crystal structures of iron alloys, metal oxides and lower mantle silicates (e.g. perovskite and post-perovskite) at high pressure and temperature, allowing further insight into the composition, temperature, and structure of the core-mantle boundary. Additionally, it's also clear that as analytical techniques advance in studying materials under high pressure and temperature, increasingly we see additional restrictions on the minimum size of samples that we can study. The nanometer spatial resolution of the NSLS II X-ray beams will enable new ground breaking work to challenge accessibility to the pressure at the center of the Earth's core (3.5 million atmospheres) and beyond. The high spatial resolution X-ray beam will also significantly enhance the capability to recognize heterogeneities of pressure, temperature, chemistry, structure and phase within small samples and to improve reliability of experimental data obtain at such high pressures. With such advances in experimental capabilities, we expect to address the long-standing issue of core composition and to understand the new observations of inner core seismic anisotropy, super-rotation and magnetism.

Evaluation of the NSLS/NSLS-II Earth and Environmental Sciences Community; Growth, Expansion, and Transition:

Existing statistics gathered by the NSLS facility since 1990 show that the percentage of users that are categorized as "Geosciences & Ecology" researchers at the NSLS have continued to grow at a rate of approximately 0.6% per year (with more rapid increases of about 1.5% per year since 2005). The community now constitutes about 17% of NSLS users, the third largest research group of the facility. Increases in subscription rates since 2005 have been largely driven by specific Earth and environmental science community initiatives jointly sponsored by DOE (BES and BER) and NSF beginning in 2003. These levels of subscription are consistent with statistics reported for this community from all four DOE operated synchrotron user facilities. The community that has frequented the NSLS consists primarily of individual university and government agency principal investigators (PIs) funded through a variety of agencies supporting synchrotron based research. These agencies include DOE (primarily through the BES Geosciences Research Program and the BER Environmental Remediation Sciences Program), NSF (through the Divisions of Chemistry, Earth Sciences and Atmospheric Sciences, Geosciences Directorate), EPA (Office of Research and Development, Superfund, National Center For Environmental Research), and USDA (Agricultural Research Service).

At all four DOE synchrotron facilities the Earth and environmental science user communities have been instrumental in the development and utilization of beamlines that support their research programs. In particular this is true for x-ray microprobe instruments, extended x-ray absorption fine structure beamlines, and beamlines constructed to support high-pressure research efforts. This has resulted in communities that have significant expertise in their successful design and operation. For some instruments the community intends to take the lead in forming Beamline Advisory Teams (BAT's) for next generation instruments at NSLS-II and in guiding their design and utilization. We summarize these efforts below by technique and individually list each beamline in detail in Table 1.

Community Beamline Utilization:
The earth and environmental science community utilizes a relatively broad spectrum of beamlines at 2nd and 3rd generation light sources. The beamlines frequented are also typically highly oversubscribed. For example, the two dedicated hard x-ray microprobes at the NSLS in cycle 2 of FY 2007 were oversubscribed by 226% overall. For x-ray absorption spectroscopy even with the availability of eight beamlines, the technique was oversubscribed by 132% for the same period. These five techniques are expected to remain the primary drivers for the next generation of Earth and environmental science experiments at NSLS-II. In addition to this suite of techniques, x-ray surface scattering techniques (such as X-ray reflectivity and grazing incidence X-ray scattering studies) have become more highly utilized by the community over the past several years at the Advanced Photon Source, and we expect they would be increasingly utilized by the MES/LTG community at NSLS-II.

Recommendations for NSLS-II:
Based on the input from the community, the following evaluation of user needs at NSLS-II is provided subdivided by technique. These sections are accompanied by a table (Table 1) which summarizes these anticipated beamline needs including an identification of optimal NSLS-II source, which of these will be new or transitioned beamlines, estimates for the minimum fraction of each beamline to be used by the community, performance needs, desired instrumentation and detectors, users that have agreed to participate in BAT's for these given beamlines, and an assessment of how critical it is to have individual beamlines operational in the 1st stage of NSLS-II operations.

X-ray Absorption Fine Structure (XAFS)

Bulk XAFS is a core competence of the environmental community and is a crucial tool to cutting edge molecular environmental sciences and low temperature geochemistry (MES/LTG). A strong grounding in bulk EXAFS spectroscopy enables the excellent development of micro- and nano-beam spectroscopy methods for our community. There are currently 8 bulk XAFS beamlines at the NSLS, all on bending-magnet sources. Of these, 1.85 effective beamlines are used for MES/LTG experiments and overall subscription is 132%. Quick EXAFS is under development at X18B, and mid-energy XAS for MES/LTG is currently conducted at X15B. There is a great deal of synergy in the energy ranges open to spectroscopy between these two instruments and the X1A STXM instrument, something that should be replicated in the transition to NSLS-II. The advanced capabilities of NSLS-II will open up new opportunities for continued and enhanced use of XAS in increasingly challenging materials. We recommend a "shared and optimized" approach to beamline involvement. Many MES/LTG applications of XAS share common requirements with those of other fields (e.g., life sciences and material science) and can be accomplished at beamlines supporting a range of capabilities, while a larger portion of MES/LTG work requires specialized beamlines and scientific staff optimized for this community.

The proposed damping wiggler based EXAFS project beamline will clearly be highly subscribed by the MES/LTG community and its exceptional brightness will push both the limits in concentration of samples that can be studied using EXAFS and the speed with which data can be collected. For our community, where natural elemental concentrations are often in the parts per million and billion ranges, improving the detection limit is a critical need. However, in addition to the DW EXAFS beamline, we estimate that at a bare minimum the MES/LTG community will require the equivalent of a full three pole wiggler (TPW) and 50% of a soft bend for bulk spectroscopy. We estimate there is enough demand for next generation EXAFS experiments to warrant the construction of approximately 3.4 equivalent beamlines for MES/LTG studies. The TPW source will fill several niches that cannot be filled by the DW – including measurements of aqueous and biological samples that will not tolerate the photon flux of the DW source. We expect the TPW and DW beamlines will be utilized heavily to their highest energies that maintain good flux. The soft bends will be relied upon for measurements up to about 4keV. All three XAS sources will need to deliver a large, stable beam suitable for the bulk components of all experiments. That said, all three sources will also need to provide a complimentary set of smaller spot sizes (while recognizing that the core XAFS experiments in MES/LTG are not driven directly to the smallest possible spot sizes). To offer an example, a study of a phytoremediative plant can use a 250 micron spot to examine metal distribution over whole-plant length scales, a 1-5 micron spot to examine the locations of metal accumulation, and a sub micron spot to examine metal distribution within an individual cell or vacuole.

It is also important to emphasize that while DW EXAFS will be vitally important for analyses requiring high flux and broad spectral range, environmental science materials are particularly sensitive to photo-induced changes in oxidation state and speciation. Heat load concerns will limit the ability of the DW to reach below the Ti edge and the high flux of the DW will preclude measurements on particularly radiation sensitive samples. For these reasons it is critical that the MES/LTG community also have access to XAFS resources developed on TPW sources. The XAFS beamlines will also benefit significantly from ring operation in top-off mode and we are confident that the beam stability requirements for the NSLS-II floor will meet MES/LTG needs.

Time is also critical for two types of applications in MES/LTG, those with time-sensitive samples and time-resolved studies of chemical/physical processes. Many MES samples are delicate and comprised of reactive combinations of solid, liquid, and organics. High flux and brightness, combined with appropriate detection, will be needed to collect high-quality XAFS data while minimizing time and exposure. Time-resolved “Quick XAFS” requires a dedicated beamline with specially designed rapid-motion monochromator and high-speed detection. Many important MES/LTG processes are ideal for QXAFS studies but their low concentrations present great challenges at currently-available facilities. The QXAFS capabilities of the existing X18B port at the NSLS continue to be developed and the community encourages this. With continued upgrades of QXAFS and detector capabilities, we feel it is likely that these components could be migrated from NSLS X18B to a focused 3-pole wiggler, an option that should strongly be considered. We would also recommend that the DWXAS project consider R&D efforts in more fully evaluating what may be required to implement QXAFS on the damping wiggler station.

Hard X-Ray Microprobe (HXRM)

There are two dedicated hard x-ray microprobe (HXRM) beamlines at NSLS, X26A and X27A, each with 60-80% of available beam time used for Earth and environmental science research. The HXRM beamlines are typically oversubscribed by a factor of 2-3X indicating that the demand is equivalent to minimally 4 full time beamlines. Both the NSLS instruments currently employ Kirkpatrick-Baez microfocusing mirrors to achieve focused spots of 5-10 µm in diameter (FWHM), i.e., near the source size limit for NSLS, over the broad energy range required by this community (2-30 keV). Clearly there is a desire in the community to pursue continued improvements in microprobe spatial resolution and capabilities as a means of extending microfocused spectroscopies to the complex chemistry observed in natural systems at the molecular scale.

We recommend three parallel microprobe development avenues for the MES/LTG community to realize this capability. First, one of the existing two HXRMs at the NSLS should be migrated to NSLS-II in order to continue to serve the existing user community and provide them with enhanced capabilities. This migration process should include continued upgrade of optics and detectors of each instrument. A particularly attractive transition plan has one of the HXRMs moving at an early stage to a 3-pole wiggler source at NSLS-II while the second continues to run at NSLS. Subsequently, the second HXRM would migrate endstation instrumentation to a proposed canted low-β straight section. An Earth/environmental/life sciences collaborative effort is underway to form a BAT for submission of an early LOI for such a proposal. To achieve the required breadth of capabilities, we propose placing the Kirkpatrick-Baez Mirror based microprobe on one of the canted undulators with an energy range between 4-25 keV, spatial resolution from 1 mm down to potentially 100 nm, and instrumentation for XRF, XAFS, XRD and fluorescence microtomography. On the second canted undulator, we will place a zone plate based microprobe with an energy range between 2-15 keV, a target spatial resolution of 20 nm, and instrumentation for XRF and XANES. Sample mounting and registry systems will be incorporated to facilitate sample transfers between the two microprobes. The unique capabilities of this highly focused x-ray probe suite will lead to far reaching advances in our understanding of complex natural systems.

The EXAFS project beamline will also incorporate microprobe capabilities for microspectroscopy. This source will be valuable for microbeam experiments particularly at higher energy than the undulator and 3-pole wiggler can reach with usable brightness. We encourage this team to pursue their plans for a microbeam capability on this beamline and work to implement a canted ID geometry (one branch bulk, one microbeam) at the earliest opportunity. It will be crucial that the MES/LTG community participate in this beamline advisory team (BAT).

The spatial resolutions potentially achievable by the hard x-ray nanoprobe project beamline also has great potential in opening new research directions in elemental nanoimaging for MES relevant materials. Given the known level of subscription by the MES/LTG community of microprobe beamlines nationally, we recommend that representatives of the MES/LTG community participate on the BAT for this beamline. We anticipate that this community will use at least 10% of the beam time on this beamline.

Special HXRM requirements include high source and optics stability for stable microbeam production, cryogenic sample stages and ancillary laboratory space and instruments for sample preparation. The HXRM runs best with the ring operated in top-off mode, i.e., fast timing experiments are currently rare. Both energy dispersive and wavelength dispersive fluorescence detectors along with 2D XRD detectors are needed for this work. Data acquisition and processing software development and standardization is important, particularly given the desirability of storing the entire collected energy dispersive spectra for each pixel analyzed and as the number of elements in array detector systems increases. These trends are rapidly increasing the size of acquired data sets and makes processing results in real time quite challenging.

Scanning Transmission X-ray Microprobe (STXM)

A molecular-level process understanding of key contaminant reactions (actinides and heavy metals/metalloids) in the environment requires us to examine contaminant adsorption/complexation and structural incorporation in mineral phases. The reactivity of structural components on these surfaces are typically sub micron in size and vary dramatically in composition, including both natural organics (e.g., humic acids and fulvic acids) and inorganic mineral phases (e.g., iron oxy-hydroxides and clays). STXM microspectroscopy techniques are invaluable in studying these small environmentally important materials and the source characteristics of NSLS-II will offer dramatic improvements in instrument brightness. The community recommends that the existing X1A1 STXM instrument at the NSLS should be migrated to NSLS-II in order to continue to serve the existing user community and provide them with enhanced capabilities. This migration process should include continued upgrade of the X1A1 zone plate optics, detectors, and spherical grating. There is also a strong desire to improve the spatial resolution towards a goal of 10 nm, which seems achievable but only with a long-term, well funded R&D effort on the fabrication of large-diameter zone plates. Nanofocusing optics for ~10 keV x-rays are part of the NSLS-II R&D plan, with an emphasis on multilayer Laue lenses which promise high resolution but which are not suited for use at lower energies or with easy energy tunability. The environmental sciences community strongly encourages efforts that have been proposed to complement NSLS-II R&D activities with the long-standing expertise of Stony Brook University in the development of higher resolution zone plate optics using the facilities of Brookhaven's Center for Functional Nanomaterials and the Joint Photon Science Institute. There is also a distinct need to be able to combine information gathered from the K edges of organic species organics and from the L edges of metals. This is best accomplished on a STXM instrument with an energy range from 200 to perhaps 2,500 eV, ideally in a single instrument. It's important to note that if we accomplish this goal, coupled with the other probe instruments proposed for NSLS-II, we will provide the globally unique ability to go from 0.2 to 25 + KeV at a single facility!

NSLS-II will also make new demands on fluorescence and phase-contrast detectors in terms of collection efficiency (so as to minimize radiation damage by collecting more of the signal) and count rate (because of the increased x-ray flux). Robust, low-noise, high efficiency detectors are needed for both photon counting and current mode measurements in transmission. Detector segmentation has great potential in making phase contrast imaging possible. Incorporation of an incident flux monitor into the order sorting aperture used in STXM may be necessary for flux normalization; this will require significant R&D.

Lastly, given the brightness of the NSLS-II source, radiation damage is a key concern, especially as spatial resolution is improved. For this reason it is essential to have at least one STXM with cryo capabilities. This is not a simple matter of putting a cooling stage on a sample mount, but rather a complete system with specimen transfer capabilities, tomographic tilt capabilities, and a low-mass stage to allow for rapid sample scanning.

Bulk Scattering and Environmental Science (BuSES)

Increasingly the Earth and environmental sciences community is moving towards utilizing national laboratory-based radiation sources for bulk scattering studies as these provide unique opportunities because of orders of magnitude increases in spatial, temporal and angular resolution. The following are growth areas: a) Combined hard X-ray microdiffraction and fluorescence for simultaneous identification of phase, composition and contaminant sorption on the µm scale; b) Scattering from environmentally relevant surfaces with nm spatial and ns time resolution – this will be particularly important for exploring surface heterogeneity and reactivity c) The use of pair distribution function (PDF) techniques in combination with XAFS to determine the local, intermediate and long-range structures and to correlate these structures with contaminant sorption/desorption scenarios d) Time resolved and in-situ measurements of reaction pathway and kinetics; e) Combined SAXS/WAXS/PDF to simultaneously explore geo-nanomaterials on the Å-nm-µm length scale during particle nucleation-ripening-growth and transformation; f) measurements under extreme conditions (pressure, temperature, acidity).

High flux over a wide range of energies and optimized optics, detectors and sample environment allows us to conceive of experiments that open up whole new areas of research, including real-time scattering to follow phase evolution as a function of time and environmental conditions (P, T, Eh, pH, fO_2 etc.). These techniques allow us to mimic the conditions under which naturally occurring and engineered materials operate, and they provide results that allow us to compare engineered samples and environments with those found in the field.

To continue to service new users of scattering it is imperative that the capacity for high energy, in situ, time-resolved scattering be increased at NSLS. The build-out of X-17-A1 and a commitment to engage the community in design and installation of environmental cells would allow the community to explore new scientific opportunities and prepare a knowledgeable user base to take advantage of the Powder Instrument Next Generation (PING) and a proposed suite of powder and single crystal instruments at NSLS-II. It is crucial that PSD and area detectors with moderate energy resolution (~200 eV) and ms time resolution, based on silicon technology, be available as soon as possible at NSLS. To take full advantage of the high energy available at PING the possibility of equivalent or better resolutions in a germanium-based detector are required. Continued support of the existing bulk powder lines (X7A and –B and X16) is vital to allow new science to blossom and to test scenarios for NSLS-II over the next seven years. The "Powder Instrument Next Generation (PING) beamline will be the only powder instrument optimized for high energy (> 40 keV) x-ray scattering in the United States. The integration of sample environments, especially for high pressure and high temperature applications, in combination with high angular resolution and/or high time resolution detection will make this instrument package unique in the inventory of synchrotron powder instruments worldwide. While comparable beamlines at APS and ESRF are for high through-put and high energy scattering respectively, PING will be a versatile instrument capable of high energy scattering in a variety of environmental cells available from day one and optimized for the instrument. The vision for the project powder beamline PING coming out of the recent combined NSLS/NSLS-II workshop on needs for the materials scattering community is summarized on the floor plan shown below. Since PING will concentrate on energies > 35 keV it is vital that the 5 - 35 keV gap for resonance powder scattering is filled. This can be accomplished by transferring one of the front-line powder instruments from NSLS, probably X-16, to a 3-pole wiggler port at NSLS-II. Chemical crystallography is served in the powder diffraction sphere by current powder beamlines at NSLS, although there are shortages of beamtime for the outside user. For routine single crystal diffraction the situation at NSLS is dire. Several synchrotrons now have single crystal efforts and they are typically successful if users are provided a mail in service that provides reliable data on a platform with which users are familiar. As soon as possible the NSLS should identify a beamline onto which a commercial single crystal diffractometer such as the Bruker Apex can be placed. Following a period of operation this beamline can be transitioned to NSLS-II.

Infrared Microspectroscopy and Imaging

There is increasing demand by the MES/LTG community for the high resolution spectroscopic information retrievable for environmental samples using synchrotron based mid- and far-IR instruments. Because IR spectroscopy is especially sensitive to vibrations of O-H, C-H, C-O, N-H, and C-N bonds, it has great potential for applications to organic compounds and the chemistry of microbes, as well as for the identification of phases and of adsorbed organic species at specially designed mineral/water interfaces (Brown and Sturchio, 2002). Additionally, instruments optimized for far IR microspectroscopy can be used to constrain mineralogy in-situ and correlate this with the organic components present in the same sample. Coupled with microfocused x-ray techniques, unique information can be gathered of how speciation of heavy metal/metalloids species is modified by the presence of organic species in the environment. This will be facilitated by specifically designing IR sample mounts that can also be used at beamlines utilizing µXAS/ µEXAFS investigation techniques for environmental studies.

Presently on NSLS U10B, the MES/LTG community utilizes roughly 30% of the available time. We fully expect that this will be the minimum community demand at NSLS-II, but we suspect there is potential for the community to utilize up to 50% of the available time on similar instrument built on a soft bending magnet source at NSLS-II. Although we recognize that the flux and spatial resolution on these soft bend instruments will be comparable to what is currently available on the existing NSLS VUV-IR instruments, the exceptional requirements for beam stability at NSLS-II has the potential of increasing signal/noise of these instruments dramatically (~ a factor of up to 100x) for IR microspectroscopy applications, which will significantly improve detection sensitivity. The community also fully encourages the continued development of the array detectors for IR imaging studies. For the MES/LTG community, these instrumentation developments hold significant interest in improving our ability to image biofilms on grain surfaces. It is our understanding that coupled with high magnification objectives, the high signal/noise afforded by the stability of the NSLS-II source, and utilization of image oversampling techniques, there is an opportunity to improve spatial resolutions to the order of 1 micrometer.

Given the variety of programs the MES/LTG community utilizes in IR spectroscopy and imaging, the following are minimal requirements for the community at NSLS-II: (1) One mid- and far-IR confocal micro-spectroscopy instrument placed on a soft bending magnet source. (2) One mid-IR imaging instrument utilizing focal plane array detector systems and high resolution objectives. We feel that continued upgrades of the U10B instrument should allow end station components to be effectively migrated to NSLS-II to continue to serve the MES/LTG user community. We also encourage continued instrumentation development in this regard.

High Pressure Research

At the NSLS currently, four experimental end stations are dedicated to high-pressure research using diamond anvil cells and large volume presses. These experiments are located at the superconducting wiggler X17 at the X-ray ring and the bending magnet U2 at the UV ring. X17B2 provides the high-pressure community with state of the art capabilities for experiments in large volume presses. Diffraction experiments at high pressure and temperature in a diamond anvil cell can be performed at X17B3 and X17C. The bending magnet beamline U2A offers the unique capability of conducting infrared spectroscopy measurements at high pressure and moderate temperatures using a diamond anvil cell. Each year, the high-pressure program at NSLS serves a user community of about 200 users from 50 national and international institutions. The current NSLS-II beamlines are currently state-of-the-art, and with planned improvements are clearly candidates for transition to NSLS-II. For example, the discussed replacement of the X17 wiggler with a new superconducting wiggler, which can be operated at reduced capabilities (limited field and/or periods) at NSLS, would then be transferable to NSLS-II. The advantages of this solution for the high pressure program at NSLS are as follows: (i) the high pressure experiments would be served by a new and reliable insertion device; (ii) the reduced capabilities of the new superconducting wiggler would be equal or superior to the current wiggler; and (iii) a superconducting wiggler, suitable for high pressure research and taking full advantage of the unique source characteristics of NSLS-II would be present at the new ring on day one. Additionally, the decision of the NSLS to build a new beamline, X17A, at the superconducting wiggler port will enable new, unique experiments ideal for investigation of disordered, nano-crystalline and amorphous materials at high pressure, and using X-ray total scattering in conjunction with pair distribution function analysis. These additional high-pressure capabilities will further strengthen the high pressure research program at NSLS and could be transferred to a high-pressure or high-energy beamline at the NSLS-II.

The small source size and the high brilliance over a large range of X-ray energies of NSLS-II will greatly benefit experiments at extreme conditions and stimulate new directions in research of materials at extreme conditions. A number of beamlines are envisioned at NSLS-II which would support high-P research efforts. We don't cover this here in detail due to limitations in space and refer the facility to Table 1 and the "Materials at High Pressure: Future directions in high pressure science and instrumentation at NSLS & NSLS-II" white paper (Ehm et al., 2008). The white paper presents plans by the community to develop a suite of high-P endstations. These would include two extreme conditions diffraction stations utilizing small pressure generating devices like diamond anvil cells (DAC) or small Paris-Edinburgh (PE) cells, located at the superconducting wiggler port. The community also identifies a need for two extreme conditions diffraction stations with large hydraulic presses to generate sample environments at extreme pressure and temperature in situations where large samples (1 mm) are required or uniform pressure and temperature are important. These systems will generally work at pressures up to about 60 GPa. The high pressure community also proposes one experimental station at a U20 undulator port which will be specialized for X-ray spectroscopy at extreme conditions. Although the energy range provided by the undulator is not ideally suited for diffraction experiments at extreme conditions, some diffraction capabilities should be available at this beamlines to allow characterization of the same sample by spectroscopic and diffraction methods. For infrared spectroscopy under extreme conditions, an NSLS-II bending magnet port with a wide gap (90 mm) dipole will prove an excellent source. It is anticipated that the current IR spectroscopy end station U2A will be further upgraded and finally be moved to NSLS-II after the shutdown of NSLS.

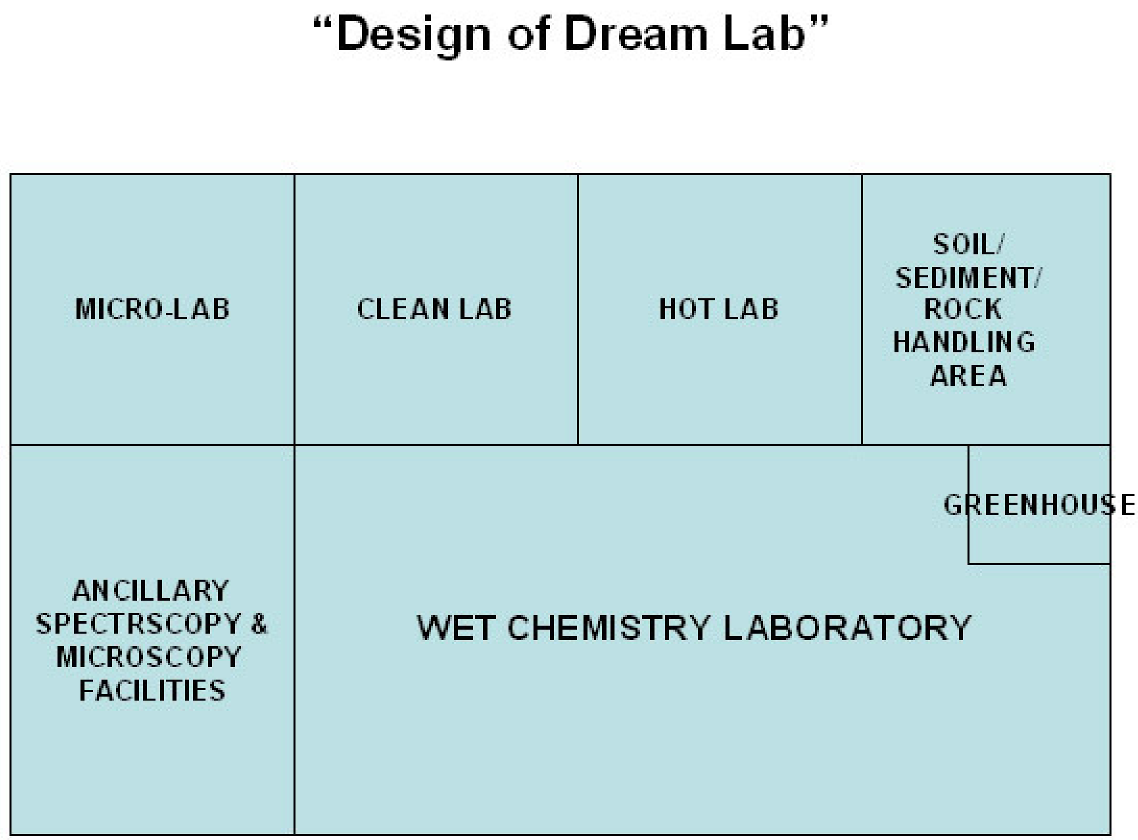
Ancillary Laboratory Requirements:

The Earth, Environmental and Life sciences user communities identify a critical need for a wide range of ancillary laboratory equipment in close proximity to endstations in order to prepare time and environment sensitive samples. Earth and environmental science users need a fully equipped geomicrobiology lab in close proximity to the beamlines. We also require a laboratory capable of handling radioactive samples. A majority of the samples that will be analyzed at the proposed x-ray probe suite do not travel well, and therefore, require on-site laboratory equipment for sample preparation, preliminary sample characterization and alignment, and special materials handling. Other needs include an anoxic glove box, centrifuge, scales, pH meters, extensive wet chemistry equipment, table-top XRD, extensive sample prep equipment, a class-100 laminar flow hood, and both petrographic and low magnification microscopes. The microscope stations should ideally integrate CCD capture devices that are networked, so that images can be directly passed to beamline endstation computers and calibrated to beamline sample stages. Instrumentation and micrococoscopy laboratories will be required to analyze samples for preliminary confirmation of the desired state of a sample (UV-VIS, RAMAN, FTIR). It would also be useful at some focused endstations to offer a large-volume anoxic sample environment (with gloves, load lock, and adequate volume to perform a wet chemistry experiment inside the chamber) in-line with the experiment. Other sample environment equipment will be needed as well (cryostat, furnace, sample change automation.) The high pressure community requires a sample and cell preparation area for diamond anvil cell and large volume press experiments. Staging and sample prep for these experiments is space intensive and requires various specialized equipment. A list of ancillary laboratory equipment is included in the appendix. The proposed scientific mission described in this white paper means that the support laboratories and instrumentation will not only benefit the Earth, Environmental and Life sciences user communities, but also these facilities will be designed to meet the needs of users conducting experiments at the interface of these disciplines.

Beamline Operations Staff

The MES/LTG community utilizes a wide variety of SR-based techniques. It will be crucial that members of the MES/LTG community participate intimately in BATs of beamlines that will be heavily utilized by this community. In addition, in our experience, users from this community benefit greatly from scientific collaborations with the beamline staff. This can be particularly beneficial when the beamline staff includes individuals with a background in molecular environmental science and/or earth science. The quality of publications is often greatly enhanced by such collaborations. Such collaborative environments are most readily developed by implementing beamlines dedicated to MES/LTG research, an approach that has been highly successful at many of the nation's SR facilities including the NSLS. We therefore recommend that the NSLS-II management seriously consider the development of MES/LTG dedicated beamlines or at a minimum include MES/LTG trained scientists in the operations teams of beamlines heavily utilized by this community.

Appendix: Schematic representation of desired ancillary lab requirements



MICROBIOLOGY

pH, DO probes
Sub zero refrigerators
Autoclaves
Culture plates
Glove boxes
UV-VIS & fluorescence spec.
Microscope
Hot plates, ovens
Water Baths
Stir plates
Cryo-facilities
Centrifuges

HOT LAB

pH, DO probes
Refrigerators
Autoclaves
Culture plates
Glove boxes
UV-VIS & fluorescence spec.
Microscope
Fume hoods
Hot plates
Water baths
Stir plates
Cryo-facilities
Centrifuge

WET CHEMISTRY LAB

pH, DO, redox probes
Balances
Glove boxes
Refrigerators
Lab accessories (glassware, filters, chemicals etc.)
Fume hoods
Hot plates, ovens
Water baths
Stir plates
Cryo-facilities
Centrifuges (at least one ultracentrifuge)

CLEAN LAB

SPECTROSCOPY/ MICROSCOPY LAB

FTIR spectrometer/microscope
Raman spectrometer/microscope
UV-VIS spectrometer
Fluorescence spectrometer
Optical & petrographic microscopes
Microtome???? EM???

SOIL/SEDIMENT/ ROCK HANDLING AREA

Clean saws for handling cores or for rock sections

Beamline Suite	Station	Beamline Type	Earth/Enviro effort or BAT participation	Optimal NSLS-II Source	New or Transition	Analytical Techniques	Estimated % of effective beamline Earth/Enviro Community may Utilize	Optimal Energy Range	Desired Monochromator/Grating	Desired Optics	Beam Size Goal	Desired Detectors	Potential BAT Members	Notes	Operational for phase:
Mid and High Energy X-Ray µprobes	Micro - 1A	Hard x-ray µProbe	Earth/Enviro	U20 Undulator (canted)	Station equipment moved from X27A	µXRF, µXAS, µXRD, fluorescence CMT	65%	4-25 keV	Si(111) &Si(311), cryogenic DCM	Si KB mirror pair, beamline mirrors to produce secondary focus at variable slit (tunable spot size)	100-1000 nm	energy dispersive arrays for XRF (NSLS/CSIRO massively multi-element array), XAFS; buffering electronics; image plates and CCDs for µXRD	Lanzirotti, Sutton, Miller, Northrup, Fitts, Reeder, Eng, Rivers, Vogt, Woloschak, Jones	collaborative effort with life sciences. Early LOI for 1A + 1B, MIE	1
	Micro - 1B	Mid-Hard x-ray µProbe	Life Sciences and Earth /Enviro Sciences joint effort	U20 Undulator (canted)	New beamline, shared infrastructure and operation with 1A	µXRF, µXAS	45%	2-15 keV	Si(111) &Si(311), cryogenic DCM, grating monochromator to reach 2 keV	hard x-ray zone plates, focal plane tracking during mono scans	20-100 nm	energy dispersive arrays for XRF (NSLS/CSIRO massively multi-element array), XAFS; buffering electronics	Lanzirotti, Sutton, Miller, Northrup, Fitts, Reeder, Eng, Rivers, Vogt, Woloschak, Jones	collaborative effort with life sciences. Early LOI for 1A + 1B, MIE	1
	Micro - 2	Hard x-ray µProbe	Earth/Enviro	TPW	Transition X26A (end-station eqipment only)	µXRF, µXAS, µXRD, fluorescence CMT	80%	4-25 keV	Si(111) &Si(311), DCM	Si KB mirror pair (transitioned from X26A), full field tomography apparatus upstream of µProbe	100-1000 nm	energy dispersive arrays for XRF, XAFS; buffering electronics; image plates and CCDs for µXRD; visible light CCD for CMT;	Lanzirotti, Sutton, Miller, Northrup, Fitts, Reeder, Jones	collaborative effort with life sciences. LOI for transitioned beamline. 2nd round LOI	2
	Micro - 3	Tender x-ray µProbe	Earth/Enviro and Life Sciences joint effort	soft bend	Transition X15B	µXRF, µXAS	50%	1-8 keV	transitioned X15B monochromator	Ni coated KB mirror pair, secondary focus (tunable spot size)	1.0-10.0 µm	energy dispersive arrays for XRF, XAFS; buffering electronics;	Northrup, Brandes, Sparks, Hesterberg, Myneni	Later LOI	2
	Nano - 1	Hard x-ray nanoprobe	Project Beamline (BAT)	U19 Undulator	New (project)	nm-XRF	10%	4-24 keV	cryo cooled Si(111)	MLL lenses	1 nm	energy dispersive arrays for XRF	Lanzirotti, Vogt, Jacobsen	Project (LOI first round)	1
Mid and Far IR µSpectroscopy	IR - 1	IR-µSpec	BAT	Soft Bend Magnet	Move U10B	Mid- and far-IR microspectroscopy	30%	50-4000 cm-1	interferometer		1.0-10.0 µm	Bolometer (far-IR), MCT-A (mid-IR)	Miller, Carr		
	IR - 2	IR-imaging	BAT	Soft Bend Magnet	Move U4IR	Mid-IR imaging	20%	500-4000 cm-1	interferometer		1.0-10.0 µm	MCT-A FPA with a spectral range from 500-4000 cm-1	Miller, Carr		
EXAFS	EXAFS - 1A	macro beam on DW	Project Beamline (BAT)	DW90	New (project)	EXAFS	30%	5.5-90 keV?	Si(111)/(333), step and slew modes	macro focusing	0.2x0.2-5x55mm	energy dispersive arrays; buffering electronics; high energy resolution, wavelength dispersive, area detector for XRD, diffractometer for DAFS		Project (initially shares beam with exafs-1B) (LOI first round for both)	1 and 2
	EXAFS- 1B	micro beam on DW	Project Beamline (BAT)	DW90	New (Project)	Micro XAS	30%	5.5-50 keV	Si(111)/(333), step and slew modes	KB optics	~1.0 µm	energy dispersive arrays; buffering electronics;		Project	1 and 2
	EXAFS - 1C	Side Station on DW	Project upgrade, multidisciplinary (BAT)	DW90	New (upgrade to Project beamline)	EXAFS	25%	2-6 keV	Si(111)	macro focusing	0.5x6-9x6 mm	energy dispersive arrays; buffering electronics;		later LOI	2
	EXAFS - 2	EXAFS on TPW	Multidisciplinary (BAT)	TPW	Transition X11A or X19A	EXAFS	50%	4-25 keV	Si(111) &Si(311)	macro focusing	0.1-1 mm?	energy dispersive arrays; buffering electronics;		Later LOI	1
	EXAFS - 3A	EXAFS on TPW	Life Sciences (BAT)	TPW	Transition X3B	EXAFS	25%	4-25 keV	Si(111) &Si(311)	sagittal focusing monochromator	0.1-10 mm	energy dispersive arrays; buffering electronics;		early LOI?	1
	EXAFS - 3B	EXAFS on TPW	Earth/Enviro and Life Sciences joint effort	TPW	New	EXAFS	50%	4-25 keV	Si(111) &Si(311)	sagittal focusing monochromator	0.1-10 mm	energy dispersive arrays; buffering electronics;		Later LOI	2
	EXAFS - 4	EXAFS on TPW	NIST (GU access)	TPW	NIST Plan	EXAFS	20%	4-25 keV	Si(111) &Si(311)		0.1-10 mm	energy dispersive arrays; buffering electronics;		early LOI	1
	EXAFS - 5	EXAFS on Soft Bend	Multidisciplinary (Earth/Enviro BAT)	Soft Bend	Transition X15B program	Tender EXAFS	50%	1-6 keV	various	macro focusing	1 mm	energy dispersive arrays; buffering electronics;	Northrup, Hesterberg, Brandes, catalysis and mat sci	later LOI	1
	QEXAFS - 1	Quick scanning on 3PW	Catalysis (BAT)	3PW	X18B transition	Quick-EXAFS	30%	4-22 keV?	Si(111) &Si(311)		1-10 mm	energy dispersive arrays; buffering electronics;		contribution to Catalysis effort; LOI, MIE;	1
	QEXAFS - 2	Quick scanning on DW	Catalysis (BAT)	DW90	New beamline	Quick-EXAFS	30%	5-20 keV?	Si(111) &Si(311)		1 mm	energy dispersive arrays; buffering electronics;		contribution to Catalysis effort; LOI, MIE;	2
Bulk Scattering - High E	PING -1	Focused beam on DW	Project Beamline (BAT)	DW100	New (project)	High res powder, time resolved, PDF	10%	40 - 100 keV	Double bent Laue	CRO	5 - 500 µm	Analyzer-bank, Si(Ge) strip, Area Interchangeable	Billinge, Chupas, Ehm, Hanson, Kaduk, Parise, Stephens	Project	
	PING -2	Focused beam on DW	Project Beamline (BAT)	DW100	New (project)	HP, environmental cells	20%	40 - 100 keV	Double bent Laue	CRO (+ KB?)	5 - 500 µm	on all three beamlines			
	PING -3	Fixed(3) energy side station DW	Project Beamline (BAT)	DW100	New (project)	Engineering, PDF, HP	20%	45 keV	Laue	KB?	5 - 500 µm				
Bulk Scattering - Low E	Bus - 1	Focused and unfocused bulk powder	Materials	3-pole wiggler	transition X7A/B/X16	High res powder	10%	5 - 20 keV	?	?	5-500 µm	Analyzer bank (like PING-1)	Billinge, Chupas, Ehm, Hanson, Kaduk, Parise, Stephens	Collaborative effort with materials	
	Bus -2	Single crystal	Materials	3-pole wiggler	New (project)	Single crystal	10%	5-20 keV	?	?				collaborative chemical crystallography	
High Pressure / High Energy	HiP - 1A	High P/E SCW	Earth/Enviro	SCW 60	New	Large Volume Press diffraction/imaging	75%	4-100 keV			1.0-10.0 µm		Weidner/Ehm		
	HiP - 1B	High P/E SCW	Earth/Enviro	SCW 60	New	LH-DAC diffraction/imaging	75%	4-100 keV			1.0-5.0 µm		Weidner/Ehm		
	HiP - 1C	High P/E SCW	Earth/Enviro	SCW 60	New	LVP diffraction/imaging	75%	30-40 keV			1.0-5.0 µm		Weidner/Ehm		
	HiP - 1D	High P/E SCW	Earth/Enviro	SCW 60	New	LH-DAC diffraction/imaging	75%	30-40 keV			1.0-5.0 µm		Weidner/Ehm		
	HiP - 2A	Inelastic Scattering		U19 CMPU	New	LH-DAC; Inelastic Scattering and Spectroscopy, Diffraction	50%	5-25 keV			1.0-5.0 µm		Goncharov, Duffy		
	HiP - 2B	Inelastic Scattering		U19 CMPU	New	LH-DAC; Inelastic Scattering and Spectroscopy, Diffraction	50%	5-25 keV			1.0-5.0 µm		Goncharov, Duffy		
	HiP -3	IR µSpectroscopy	Earth/Enviro	Soft bend	Transition U2A	High-P mid and far IR µSpectroscopy	50%	50-4000 cm-1	interferometer		1.0-10.0 µm		Zhenxian Liu		