Development of a Medium-Term (5 year) Plan
for APS Beamline Improvements and Enhancements

Introduction:

Over the next several months, the APS staff, users and management will be developing a plan to position the APS for the years leading up and into a potential upgrade of the facility. The plan is broad and includes accelerator as well as beamline upgrade plans that will keep this facility competitive to perform world-class, cutting edge science. The goal is to create a prioritized agenda so that, even with limited funds, we can make sound strategic decisions on how available funds should be invested. This memo specifically addresses the development of a medium-term (5 year) beamline upgrade plan that will dovetail seamlessly with APS's long-term upgrade plan (which at present is the integration of an energy recovery linac into the existing APS infrastructure).

The Process:

The focus of this process will be to develop a medium-term plan for improvements and upgrades of beamlines at the APS. A parallel process will develop a medium-term plan for the accelerator with the idea that these two plans will be merged to create a strategic investment plan for the entire facility.

We are asking both XSD- and CAT-staff to contribute to the APS plan by developing a strategic plan for beamlines, which could include new/additional insertion devices, optics, detectors, and scientific software. Of key importance is that the proposed improvements and/or enhancements are driven by the quality of x-ray science that will be enabled. The proposal must specify:

1. what new capability or technique the upgrade will enable, and
2. how the new capability/technique will impact science and the science community

(A complete list of points that should be addressed in any submitted upgrade proposal is given in Appendix A.) The proposal associated with a given beamline should be no longer than 4 pages.

XOR staff will solicit input and advice from the newly formed Beamline Advisory Groups (BAGs) to develop a list of improvements and/or enhancements that are required and cost estimates to complete the tasks. After the list has been developed, it should be sent back to the BAG to review and comment. A similar process will be requested from the CATs, in this case input and advice should be received from the CAT membership, CAT science or technical advisory committees, and/or the user community the CAT serves.

The Time-line:

We would like the beamline proposal from XOR and the CATs by March 28, 2008. The proposals should be e-mailed to Dennis Mills – dmm@aps.anl.gov (and cc'd to George Srajer srajerg@aps.anl.gov and Gabrielle Long gglong@aps.anl.gov). The individual contributions will be assembled into a draft APS improvement plan and be presented for discussion at the APS User Meeting in May 2008. Using the input gathered at the User Meeting, the draft plan will be refined and ready for discussion and project prioritization at the APS Retreat scheduled for October 20 and 21, 2008.

The Result:
The result of this exercise will be a prioritized list of improvements/enhancements that need to be undertaken to the accelerator and beamlines to keep the APS scientifically competitive over the next 5 years (or more). As funding becomes available, we will invest in the projects based on this list, and update the list as needed.

Questions:
Feel free to contact Dennis Mills (630 252-5680 or dmm@aps.anl.gov) if you have questions.

Appendix A

The justification for the proposed upgrades should address the following points:

- The Science that will be impacted
- Added value of the Mid-term Upgrade
  - smaller samples
  - better spatial resolution
  - higher temporal resolution
  - higher throughput
  - etc …
- Expected user communities
- Enabling technology and infrastructure
- Partnerships
- Industry and technology transfer

In addition, a budgetary profile for completion of the proposed upgrade should be included.

Appendix B

Example of a proposed beamline upgrade:

Frontier science using a new laser-initiated time-resolved x-ray facility for photochemical research at beamline 11-ID-D

Science

This proposal is linked to the BES Grand Challenges Report "Directing Matter and Energy - Five Challenges for Science and the Imagination" through its ability to offer input to the first two of the five questions that are posed, "*How do we control material processes at the level of electrons?"* and "*How do we design and perfect atom- and energy- efficient synthesis of revolutionary new forms of matter with tailored properties?"*

Fundamental breakthroughs in chemical reaction theory and control require not only knowledge of static structures of reactants and products, but also resolution of time-dependent atomic positions of these molecules along reaction coordinates to visualize the structures of transient states that are critical for determining…..

The goal of the research program at this facility is to understand the molecular structural basis of photochemical reactions (such as photoinduced electron transfer, energy transfer, and solar energy conversion in non-crystalline media) on time scales from tens of picoseconds to microseconds by imaging molecular coordinates as a function of time after photoexcitation along the reaction path. The increased beam time available at the upgraded facility will also benefit research programs in electrochemistry, photo-catalysis, hydrogen production, and fuel cells. In addition to addressing two Grand Challenge areas, the proposed upgrade will greatly enhance research capabilities to help meet two of the four long term goals in BES Program Assessment Rating Tool Performance Measures issued by the Office of Management and Budget, which are to "demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications" and to "demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems." The proposed upgraded Laser-Initiated Time-Resolved (LITR) x-ray facility will provide a unique characterization tool to rationally design, model, and analyze materials, including polymers and biomaterials on a nano-scale, for energy related applications……

Added value of the medium term upgrade

We propose to upgrade the existing Laser-Initiated Time-Resolved X-ray Absorption Spectroscopy facility that was originally established through a New Facility Initiative Grant from DOE. The new facility will be significantly more efficient and versatile for a growing user community in time-resolved x-ray sciences. Pioneering LITR-XAS experiments have been successfully carried out at the existing facility since 2000. More recently, we have successfully carried out Laser-Initiated Time-Resolved Wide Angle X-ray Scattering experiments at the……

The new x-ray facility upgrade will reduce the required acquisition time by 2 - 3 orders of magnitude, will enable time-resolved experiments to be scheduled for 80% of the available time (as opposed to the current 20%), and will allow a wider range of sample systems to be studied. Table 1 summarizes the various enhancements expected from the upgrade.

Table 1. Enhancement factors for LITR-XAS/WAXS experiments with the upgrades

UPGRADE	LITR-XAS	LITR-WAXS
Beamline insertion devices and optics	Photons/bunch 10-50 times higher	Photons/bunch 100-500 times higher (another factor of 100 for polychromatic beam)
Laser	Repetition rate 10 times More selections in excitation wavelengths	
Röntech Detector Arrays	Total count rate 3 times Usable beam time 4 times	N/A
Pilatus Detector Arrays	N/A	Signal to noise ratio
Total estimated enhancement factor for an individual experiment	Up to 500	2000-4000

Expected user communities

As an indicator of the wide spread, multidisciplinary interest in new basic research opportunities offered by the proposed LITR-XAS/WAXS capabilities, we have received letters of support from more than ten groups (see "Partnerships and user interest") who intend to be among the first users of this facility. We expect the demand for time resolved x-ray experiments to grow further in the future…..

Enabling technology and infrastructure

Three key components of the LITR-XAS/WAXS instrumentation are to be upgraded by this proposal:

- An ultrafast 10-kHz repetition rate laser system ($570K) will replace …..
- A 21-element silicon drift detector array ($400K) will replace…
- A fast pixilated PIN-array detector unit ($600K) will replace …

The proposed laser and detector systems are highly optimized for time-dependent experiments and will allow bunch-to-bunch time resolution in the standard 24-bunch mode without the use of an x-ray shutter. The facility will form the basis for a general user community dedicated to the investigation of charge transfer and structural time dependent effects in non-ordered materials.

Partnerships and user interest

Benjamin Gilbert: Staff Scientist, Lawrence Berkeley Laboratory
Glenn Waychunas: Staff Scientist, Lawrence Berkeley Laboratory
Michael D. Hopkins: Professor & Chair of Chemistry Department, University of Chicago
Joseph T. Hupp: Professor & Chair of Chemistry Department, Northwestern University
Himanshu Jain: Professor of Materials Science, Lehigh University
Frederick D. Lewis: Professor of Chemistry, Northwestern University
Jonathan S. Lindsey: Professor of Chemistry, North Carolina State University
Gerald J. Meyer: Professor of Chemistry, Johns Hopkins University
Martin Newcomb: Professor of Chemistry, University of Illinois
Russell Schmehl: Professor of Chemistry, Tulane University
Michael Wasielewski: Professor of Chemistry, Northwestern University

Industry and technology transfer

None foreseen at this time.

Estimated Budget:

	Year 1	Year 2	Year 3	Year 4	Year 5	Total
M&S	$50K	$100K	$75K	$50K	0	$275K
Capital	$570K	$400K	$600K	0	0	$1570K
Total	**$620K**	**$500K**	**$675K**	**$50K**	**0**	**$1845K**