Scientific needs for future X-ray sources

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1 1-page summary of the workshop

This document is the result of the "Science needs for new X-ray sources" working group at the 48th ICFA Advanced Beam Dynamics Workshop on Future Light Sources. The charge to this working group was to identify the photon source properties required to deliver breakthrough science beyond what can be achieved using currently existing X-ray light sources (including sources currently under construction). We asked participants to identify a set of broad areas of scientific research that would benefit from breakthroughs in light source technology, identifying the first experiments in a range of disciplines, and from this determined the photon source properties required to deliver new science. We therefore focused on the science areas, identified key first experiments in each area, and then looked for commonality in light source properties across different science areas.

A common theme from the workshop is that the next frontier in breakthrough science will be achieved by a transition from static studies to time-resolved studies of material behavior, chemical reactions and biology. Complex time resolved studies need sources with pulses on demand and time sequences tailored to individual experiments, and this is difficult to do at current storage ring based sources.

It is clear that no one new light source facility can serve the needs of breakthrough science in all areas. However across a range of science applications we found that there was a strong need for the following three broad classes of new light source:

1. Ultra-short pulse, high peak power X-ray source
Studies of the time-resolved dynamics of electrons and atoms require very short pulses to generate ‘snapshots’ of materials and chemical reactions. X-ray wavelengths must be tunable across atomic resonances in the 200 eV - 15 keV photon energy range and be able to resolve spatial scales from nanometers to atomic resolution. Peak power matters more than average brightness or repetition rate. Transverse and longitudinal coherence is required as well as the ability to customize X-ray pulse duration and repetition rate on an experiment-by-experiment basis. There should be enough single shot power for single-shot measurements, programmable pulse trains, pulse shaping, ability to serve multiple users, and the ability to synchronize X-rays to fs visible pump lasers.

2. Picosecond, high peak power very hard X-ray source
Studies in mesoscale dynamics cover micron to mm length scales and would benefit greatly from a pulsed harder X-ray source that would enable time resolved studies on bulk materials. Picosecond X-ray pulses are adequate due to the larger length scales involved, however the X-ray energy regime should cover at least 30 – 100 keV, and possibly up to 150 keV for certain experiments. Peak power matters more than average brightness or repetition rate. Monochromaticity and both transverse and longitudinal coherence are required for most analytical techniques, as well as the ability to customize X-ray pulse duration and repetition rate on an experiment-by-experiment basis. X-rays must be synchronisable with drive lasers for time-resolved studies.

3. High-flux, high-brightness quasi-CW X-ray source
Techniques that demand high monochromaticity benefit from the stability and narrow bandwidth offered by CW or quasi-CW light sources. X-ray wavelengths must be tunable across atomic resonances, and at least in the range from 200 eV to 15 keV to cover interesting atomic resonances and resolve spatial scales from nanometers to atomic resolution in X-ray scattering experiments. High average brightness matters more than peak power and multiple simultaneous users can be accommodated simultaneously. Any technique that requires a monochromator immediately derives benefit from a stable narrow band source, where increased flux speeds up data acquisition.
2 Introduction

This document is the result of the working group “Science needs for new X-ray sources” which formed part of the 48th ICFA Advanced Beam Dynamics Workshop on Future Light Sources hosted at SLAC National Accelerator Laboratory from 1-5 March 2010. The charge to this working was to identify the photon source properties required to deliver breakthrough science beyond what can be achieved using currently existing X-ray light sources (including sources currently under construction).

The ICFA workshop series is primarily a forum for discussing accelerator and light source technology; however the light source designers and builders need input from scientists on what new light source properties are required to deliver breakthrough science. This serves two purposes: (1) it guides light source designers as to the most critical X-ray photon properties desired by scientists, which in turn guides direction of technology development; and (2) provides input to management proposing new or upgraded light source facilities on the areas of potential breakthrough science enabled by new light source technology, and the key photon source properties required to open up entirely new frontiers in science.

This document is the written report of the Science Needs working group at ICFA 2010. Naturally any document attempting to summarize a complex field into a short document runs the risk of over-summarizing a complex field, and this is particularly the case when summarizing the most pressing needs for future light sources. It is important to note that the contents of this document only reflect the input of the authors present at the workshop and are therefore not meant to be comprehensive with regards to all future science needs. We hope that this document will nevertheless be of value to the future light source and accelerator communities.

3 Organisation

The Science Needs working group was charged with identifying key breakthrough science areas that could be enabled by new light source properties not currently available anywhere in the world. We therefore asked participants to identify a set of broad areas of scientific research that would benefit from breakthroughs in light source technology. For each of these areas we asked participants to identify the breakthrough first experiments they would like to perform as well as the scientific impact of those experiments, without regard to limitations of current light source capabilities. Finally the X-ray light source properties required to achieve those experiments were identified and common themes between different research areas identified. The goal of this approach was to elucidate the photon source properties required to deliver new science by first focusing on the science areas, identifying key first experiments in each area, and then looking for commonality in light source properties across different science areas.

The goal of this working group was not to provide scientific justification for any one source – this has already been documented in detail by many technical design reports for proposed facilities. Rather we aimed to identify which photon source properties are desired to deliver breakthrough science across a range of different science interest areas, irrespective of what type of facility may be required to deliver those photons.

To provide some order to discussions working group discussions we first identified 8 science driver areas that could be advanced through the development of new science areas. Specifically:

1. Understanding Chemical Reactions
2. Molecular Movies
3. Atoms to Materials
4. Multi-component materials
5. Strongly correlated materials
6. Materials at the mesoscale
7. Matter in Extreme Conditions
8. Hierarchical Biology
As with any list the divisions are somewhat arbitrary, however our goal is to identify common photon source needs across all science areas, thus the main concern is not where the boundaries are drawn but rather that key science driver areas are represented somewhere and their photon source requirements identified.

4 First experiments in breakthrough science areas

The following section contains summaries of the science motivation, first experiments, and photon source properties required for new experiments in each of the science driver areas.

4.1 Understanding Chemical Reactions

Peter van der Meulen, Jinghua Guo, Ryan Coffee

Traditionally, the study of chemical reactions on a femtosecond or picosecond timescale has been carried out using non-linear optical techniques involving ultrashort (fs or ps) laser pulses in the ultraviolet, visible or near infrared part of the electromagnetic spectrum. The time resolution that can be obtained in these experiments is excellent, but the interpretation of the collected experimental data is often far from straightforward. This is directly connected with the wavelength of the laser pulses used: they typically induce transitions between the HOMO and the LUMO of the molecules under investigation. These molecular orbitals are delocalized over the entire molecule, making it hard to unambiguously identify a particular spectral change with, say, the cleavage of a specific chemical bond, in a complex reaction sequence.

With the advent of short-pulse X-ray lasers this major difficulty can be overcome as the properties of the X-rays often allow for a much easier connection between the experimental data and the reaction mechanism, either directly in a scattering-type experiment in which the atomic positions are imaged immediately or indirectly in which the sensitivity of spectroscopic information to the local environment is employed (chemical shift). X-ray spectroscopy can also provide the information of HOMO and LUMO with atomic (element) specific characters. In this way, the availability of intense femtosecond X-ray lasers that can be tuned between approximately 0.1 and 10 nm (to cover B and C K-edges and S L-edge) will no doubt revolutionize the field of femtochemistry.

Furthermore, it is expected that the pulse length of these new light sources can and will be pushed down well into the attosecond regime. This will open up new fields in chemistry in which one focuses on the motion of the electrons instead of on the motion of the nuclei: the transition from femtochemistry to attochemistry. The interest in this field is immediately obvious because electrons are held responsible for the chemical bond. The first experiments of this type will most likely concentrate on electronic wave packets in atoms, but no doubt they will be extended to individual molecules and, later on, even to condensed matter samples.

As in ordinary femtochemistry, various non-linear optical techniques can be used to study chemical reactivity using X-rays. The conceptually easiest to understand is probably the one in which an external light pulse (Infrared, visible, ultraviolet or THz) induces a particular reaction while its progress is monitored by an X-ray pulse that can be send in at an arbitrary time delay (pump-probe spectroscopy). However, even other non-linear optical techniques such as surface-enabled harmonic generation, the two- and three-pulse photon echo, transient grating and similar types of four-wave mixing spectroscopy carry great potential.

A typical test experiment to initiate the field of femtochemistry with X-ray pulses will probably involve a ‘simple’ bond-breaking reaction such as the photochemical cleavage of the central bond in gaseous molecules such as NaI and I₂. These molecules have been studied extensively using femtosecond UV/VIS laser pulses and should serve as benchmarks for the establishment of the new technique. In solution, a molecular ion as I₃⁻ would form an ideal candidate for study. Later on, one might look at more complex reactions, such as photochemical ring closures or openings in organic compounds or the photo-induced release of ligands such as...
CO from inorganic metal complexes. A particular interesting topic would be the observation of so-called conical intersections which are expected to play a very important role in multidimensional systems.

A very important subsection of chemical reactions are those taking place at surfaces. These include industrially important reactions that are mediated with the help of a catalyst such as the Haber-Bosch process, but also those occurring at the surface of small grains of dust in the upper atmosphere. X-ray femtochemistry forms an ideal tool to investigate these processes in more detail. For example, one might imagine a CO molecule bound to the surface of a catalyst. The cleavage of the C=O bond can then be initiated with an infrared laser pulse, directly exciting the C=O bond, or a THz pulse exciting the generally weaker bond between the catalyst and either the C or the O side of the CO molecule. The ensuing dissociation process can then be elucidated in great detail with an ultrashort X-ray probe pulse using a wide variety of well-established techniques such as XAS or RIXS or ARPES (on the catalyst), but also using X-ray correlation spectroscopy which allows one to observe changes at the catalyst’s surface with very high temporal and spatial resolution.

Another topic that has attracted, and will continue to attract, are the structure and dynamics of liquid water. In particular in biologically relevant processes such as the folding of a newly synthesized protein, the surrounding water molecules are considered to be of critical importance. The dynamical response of the various hydration shells surrounding the protein may, perhaps, be compared to the dynamics and the structure of water molecules confined in small structures such as inverse micelles, tubes or Zeolite pores, which probably are somewhat easier to investigate. The results for these systems will, of course, have to be compared to the results obtained in liquid, bulk water. An especially interesting and promising experiment would be the two- or three-pulse photon echo on the oxygen π* resonance which would provide information on the hydrogen bond breaking and making on a femtosecond and picosecond timescale for the various water molecules (bulk, confined or attached to a surface).

There is also a great interest in developing rechargeable lithium batteries with higher energy capacity and longer cycle life for applications in portable electronic devices, electric vehicles, and implantable medical devices [M. Armand and J. M. Tarascon, Building better batteries, Nature 451, 652-657 (2008)]. The present lithium-ion battery technology is based on the reversible intercalation reaction discovered in the early 1980s for both the cathode (Li$_x$CoO$_{2}$; 0 < x < 1) and the anode (Li$_x$C$_6$; 0 < x < 1). This technology is widely used for portable electronic devices because its energy density is much higher than that of any other conventional rechargeable battery system. The specific energy density is now twice as large as that of the first product, an advance principally due to technical efforts towards efficient packing of components inside a cell rather than material innovations. However, such a development strategy has gradually sacrificed the safety margin and increased the risk of explosive accidents initiated by abrupt oxygen extraction from the charged cathode at elevated temperatures. Reduction in cost has also been restricted by the requirement of a large amount of cobalt in the cathode material. Safety and cost are critical issues and have prevented lithium-ion batteries from being used for large-scale applications.

Several challenges need to be met before these expectations can be realized because lithium-ion batteries currently do not meet the application requirements for use in transportation or as backup for renewable energy sources, applications where exponential increases in electrical energy density are still necessary. Yet these changes cannot come with a penalty in terms of device safety and cycle life of the device, which implies that the mechanisms of their reaction with lithium need to be well understood in order to locate possible sources of failure.

Particle size, shape, surface composition, and surface structure are key factors controlling catalytic performance of nanoparticles (NPs). However, the properties of NPs are usually difficult to characterize at the atomic level under practical catalytic conditions, especially when the size of NPs is below 1 nm [C. A. Witham, W. Huang, C.-K. Tsung, J. N. Kuhn, G. A.
Somorjai, and F. D.Toste, Converting homogeneous to heterogeneous in electrophilic catalysis using monodisperse metal nanoparticles, Nature Chemistry 2, 36 (2010)]. Recently, new synthetic methods were developed for generating mono- and bimetallic NPs with sizes ranging from less than 1 nm to about 10 nm. The catalytic activity of these NPs for CO oxidation and ethylene hydrogenation under atmospheric pressures was investigated.

Finally, extremely high brightness sources enable one to exploit the special properties of so-called two-site, double-core hole states. It has been shown that these states show a much larger chemical sensitivity (chemical shift) than the ‘ordinary’ single-core hole states which may be of great help in identifying the different species participating in a reaction. On the fundamental side, differentiating charge migration (flow) from charge transfer (hopping) in the valence state can potentially be resolved by the photoelectron spectra of two-site double core holes. Such double-core excitations can only be produced at x-ray FEL sources where the absorption cross-section times the photon density approaches unity. For second row elements, this calls for ca. $10^{12}$ photons in the 200-800eV energy range since absorption cross-sections are on the order of mega-barns. Potentially near-degeneracy two color x-ray pulses that can be timed within the characteristic Auger times (~ 5fs) would be very useful for this novel new spectroscopy, that might be designated x-ray two-photon photoelectron spectroscopy (XTPPS).

**Photon needs:**

The following new source parameters would be desired for time-resolved femtochemistry studies:

- 1-50 fs pulses (with some experiments demanding pulses as short as 100 as)
  - Auger time ~5fs, photoelectron times in a
- 100 eV to ~10 keV photons (not necessarily all at the one facility)
- Monochromaticity, tunable to resonances
- High peak X-ray intensity
- Pulse trains on demand (ideally different pulses to different experiments)
- Flexibility in bunch structure, pulse structure
- X-ray pulse shaping similar to optical lasers, chirping (chirped adiabatic passages)
- Rep rate of source commensurate with 10 fs optical pump lasers (<10kHz)

Experiments in femtochemistry require 1-50 fs pulses and high peak intensity for non-linear experiments involving only X-ray pulses. For X-ray probe pulses (external source initiates the reaction) maybe a lower peak intensity can be tolerated. XAS probe pulses may be fairly weak and high repetition rate is more important (especially when risking space charge). The same applies to RIXS measurements, which is very photon hungry experiment. For XCS the transverse and longitudinal coherence is critical, which probably also holds for the non-linear X-ray experiments. Intensity requirements for the non-linear X-ray experiments are hard to give just now, in the absence of accurate non-linear material parameters. Extending these experiments into the regime of attochemistry – enabling the time-resolved study of valence electrons responsible for chemical reactions – requires the generation of even shorter pulses on the order of 100 as duration.

The working group observed time resolved experiments are hard to execute at synchrotrons. The single bunch, lower average current provided in single-bunch synchrotron operation makes other customers unhappy, whilst the low average flux means that experiments take too long for the many time steps required in time-resolved studies – experimenters need more flux, more flexibility in mode of operation, and better detectors to make use of every pulse. Furthermore, different time resolved studies need different pulse structures – some systems require intense pulse every 100ms, whilst other experiments need more frequent pulses. It is challenging to perform time resolved experiments at a storage ring source where
the same parameters are delivered to all users at the same time – pulse frequency selectable on an experiment by experiment basis is strongly desired.

4.2 Time-resolved movies of molecules in action

An overarching grand challenge for chemical science is to be able to design, engineer, and ultimately control interactions at different scales for synthesizing desired chemicals and materials. Energy relevant chemicals and materials are a key forum for this fundamental science and provide many societally useful and scientifically challenging ventures. Conversions of feedstocks such as biomass and CO₂ into desired products such as fuels and fuel precursors is one such example and require selectively breaking and making bonds. In addition, these transformations as well as interconversions of electrical and/or solar energy to chemical energy involve multi-step mechanisms that often require coupling of these bond breaking/making processes with electron transport and transfer to help drive energetically uphill processes. Designing catalysts for these processes requires identifying and controlling processes at active sites, learning how to link processes at multiple sites, and controlling the environment of the processes to facilitate the reaction and transport processes in these multi-step mechanisms. Traditional synthetic approaches, which rely on high heat treatment, mechanical or chemical mixing, lack the required spatial and structural control.

One approach to developing complex catalysts begins with the design of catalytically active sites at the molecular level. New high-resolution imaging tools must be developed to allow observation of reaction processes under operating conditions (at pressures, temperatures, and other conditions relevant to catalytic reactions) to develop an understanding of how the underlying catalyst structure, affects the operation of the catalytic process. The dream of a molecular movie of a reactant undergoing chemical transformation at an active catalyst site captures the time, spatial, and selectivity drivers of what is needed. One important caveat emptor is quantifying how severely one is perturbing the system you are probing with such intense, short photon pulses.

Photon needs:
The new source parameters required for making time-resolved movies of chemistry are very similar to those required for femtochemistry studies. Specifically:
- 1-50 fs pulses (some experiments would require pulses as short as 100 as)
- Auger time ~5fs, photoelectron times in as
- 100 eV to 8 keV photons
- Monochromaticity, tunable to resonances, transverse coherence
- High peak X-ray intensity, in other cases high average power
- Pulse trains on demand (ideally different pulses to different experiments)
- Rep rate of source commensurate with 10 fs optical pump lasers (<10kHz)

Catalysts undergo structural and electronic change during use; extending time-honored spectroscopies used in catalyst studies to at-pressure, at-temperature conditions with exquisite time and spatial resolution is desired. Methods that would track these changes with chemical specificity include time-dependant core-level photoemission and x-ray emission spectroscopies. Time scale demands for these experiments are as stringent as those for IXS microscopy, but initially can be relaxed. Nanometer spatial resolution with the ability to penetrate at least microns of material is needed. There is a dual demand for high spatial resolution as well as time-resolution for these experiments with demands for high-average power initially.

Production of real space single-molecule movies of catalysts with nanometer scale resolution will require methods such as: inelastic x-ray scattering microscopy. This drives the need for transversely coherent x-rays with nanometer or shorter wavelengths. In this instance, time scales are on the order of 0.1 – 1000 fs, and nanometer spatial resolution with the ability to penetrate at least microns of material is needed – in order to perform the real-condition imaging. There is a dual demand for high spatial resolution as well as time-resolution for these experiments. These experimental requirements demand high peak power photons.

### 4.3 Atoms to Materials

*Hans Beijers and Fulvio Parmigiani*

Inorganic and organic mass selected clusters represent an important and undisclosed state of the matter bridging the physical and chemical properties from single atoms to the bulk.

The present day’s demand for nano-scale devices operating at ultrafast time scales requires a deep knowledge of the matter consisting of tens or hundreds atoms. This demand sets the path for observing the evolution of both the electronic and geometrical structure versus the cluster size. In particular, these experiments will allow studying the build-up of the long range electronic structure properties from the atomic shells, along with the dependence of the collective properties and phase transitions versus the number of atoms in the clusters.

Performing these studies require spectroscopy in the energy and time domains. However, the low density matter in mass-selected cluster beams necessitates a very high photon fluxes, in the soft and hard X-ray regime, delivered in ultra-short (fs-as) pulses with variable polarization and high coherence. The up-coming accelerator-based radiation sources will fulfill these challenging needs of these cutting-edge studies at edge of our knowledge. The expected results will be of paramount importance for catalysis, electronics and magnetic materials and processes.

1- Geometrical structure (at equilibrium and off-equilibrium) of mass-selected clusters in real space and real time.
2- Phase transitions in mass-selected clusters: melting, metal-insulator (semiconductor) phase transitions, magnetic phase transitions.
3- Collective vibrations of gas clusters
4- Cluster properties and non-equilibrium thermodynamics at the femtosecond time scales
5- Chemistry of molecular clusters and nanocrystal interfaces
6- Studies of matter at ultracold temperatures HeLi um NanoDroplet Isolation (HENDI)

Photon needs:
These experiments require very bright sources of X-rays to get any measurable signal. Specifically:

- Photon energy range (from EUV to Hard-x-rays) 10 eV - 10 keV
- Photon flux > $10^{14}$ ph s$^{-1}$ mm$^{-2}$ mrad$^{-1}$ 0.1%bw
- Coherence full transversal and FTL
- Polarization Circular and Linear (variable)
- Tunability fast (1 kHz)
- Pulse duration from as to ps (possibly variable)
- Beam stability (intensity) high
- Beam stability (energy) compatible with FTL
- Pulse to pulse jitter < 500 as
- Beam divergence diffraction limited
- Repetition rate from ~10 Hz to ~1 MHz

The intensity available at the current 3rd generation synchrotron radiation facilities is still way below what would be required for meaningful mass-selected clusters experiments. This is due to both the low target densities that can be obtained in size-selected particle beams as well as the incompatibility of the time structures of particle and synchrotron beams, resulting in a low duty cycle of such experiments. Current experiments are thus mostly limited to clusters deposited onto surfaces, where the surface in most cases has a strong influence on the results. In rare cases neutral clusters in gas phase without size-selection could be studied, which again strongly limits the significance of the data. The combination of size selective spectroscopy with intense light from sources such as those provided by FEL sources will therefore allow measurements of unprecedented significance and will undoubtedly lead to a deeper understanding of the electronic structure of nanoscale metals and semiconductors, as well as of electron correlation effects in solids in general.

4.4 Multi-component, multi-functional materials:
Emergent energy applications require the design and synthesis of novel materials not only with precise control of the structures on multi-length scales, but also with multi-functional mechanical, electro-optical or chemical properties that cannot be derived from a single material or from mere homogeneous mixtures of materials. Traditional synthetic approaches mostly rely on high energy heat treatment, brutal force mechanical or chemical mixing that lacks precise spatial or structural control; or else on methods that cannot be applied on large scales. The development of the scientific principles for large scale synthesis of multifunctional materials must address three grand challenges:

1. Bottom-up synthesis methods to produce materials with controlled structures and functions from molecular to nano-, micro- and macroscopic scales;
2. Control and optimization of the properties derived from complex, multicomponent, multiphase materials and systems; and
3. Scientific and systematic approaches for rapid, reliable materials synthesis on large scales.

There is an urgent need to develop the in-situ, real-time capabilities for direct imaging and spectroscopic interrogation of the structural changes during synthesis and use of these multi-component materials. Example applications include: nanoporous material characterization and
in-use, in-situ structure determination for multi-component battery, carbon capture and sequestration, and photovoltaic materials.

Generating real space maps of multi-component materials with nanometer scale resolution will require methods such as: coherent diffractive imaging, tomographic methods. This drives the need for transversely coherent x-rays with nanometer or less wavelengths. In this instance, time scales are on the order of microseconds, but nanometer spatial resolution with the ability to penetrate at least microns of material is needed – thus demanding high average power photons.

Many of these materials undergo structural and electronic change during use. Methods that would track these changes include time-dependant SAXS and core-level photoemission and x-ray emission spectroscopies. Time scale demands for these experiments are on the order of ps to microseconds, but nanometer spatial resolution with the ability to penetrate at least microns of material is needed. There is a dual demand for high spatial resolution as well as time-resolution for these experiments.

Photon needs:
The new source parameters required for studying multi-component materials are as follows:

- 1-50 fs pulses
- 100 eV to 8 keV photons (penetration required, but also tenability)
- Monochromaticity, tunable to resonances, transverse coherence
- Transverse and longitudinal coherence for diffractive imaging
- High peak X-ray intensity for single shot measurements
- Pulse trains on demand (ideally different pulses to different experiments)
- Rep rate of source commensurate with optical pump lasers (<10kHz)

4.5 Strongly Correlated Electron Systems:
Wei-Sheng Lee (SIMES, SLAC), Jinghua Guo (LBNL), Fulvio Parmigiani (Elettra)

Many fascinating phenomena exhibited by correlated materials are known as “emerging”, phenomena that spontaneously break the symmetry of the original Hamiltonian. The “emergence” of novel phases in correlated materials, such as unconventional high temperature superconductivity, colossal magnetoresistance, and multi-ferroic behavior in
cuprates, manganites, ferrates, graphene, and topological insulators, for example, derive from strongly intertwined spin, charge, orbital, and lattice degrees of freedom. To understand these complex phenomena at microscopic level, it is often desired to measure the low energy excitations of the electronic states (~0.05 meV – 500 meV) in energy, momentum, and time domains, when the system is either in equilibrium or being driven out-of-equilibrium. The knowledge learned from these correlated systems is not only fundamentally important to our current understanding of Physics, but also can feedback to material synthesis and device engineering for new applications.

Up to date, photon-electron-out and photon-in/photon-out spectroscopies have been widely used in the 3rd generation synchrotron facilities to study the correlated electron systems (shown in Figure 1). However, due to the limit of the current light source, additional information from these techniques can be further obtained when the future light source becomes available. In following sections, we identify a few selected examples of photon-in-electron-out and photon-in-photon-out spectroscopy.

Because of the multiple techniques employed for studying strongly correlated materials, for this section we split out the photon source requirements for strongly correlated electron systems according to analysis technique.

**Photon-in-electron-out Spectroscopy**

For example: Time-Resolved and Angle Resolved Photoelectron Spectroscopy (TR-ARPES), Time-Resolved and Spin Resolved ARPE (TR-SR-ARPES), nano-ARPES

Two recent papers have shown that it is possible to control the electronic phase of a manganite by mode-selective vibrational excitation [M. Rini et al, Nature 449, 72 - 74 (2007)] and to measure the ultrafast electron relaxation in superconducting Bi$_2$Sr$_2$CaCu$_2$O$_{8+delta}$ by time-resolved photoelectron spectroscopy [L. Perfetti et. al, Phys. Rev. Lett. 99, 197001 (2007)]. An interesting playground is to study the breathing of the Fermi surface in K$_3$C$_60$ (Fig 4) and similar system by exciting the structure through selective mode vibrations [Science, 300, 2003].

**Ideal Source for TR-ARPES:**

- control of the photon density per pulse
- control of the repetition rate (from few kHz to 10 MHz regime)
- control of the polarization
- Tunable photon energy between 10 eV and ~10 keV
- pulse duration (sub fs and fs)
- Tunable “pump” photon sources: in addition to the conventional optical pump, photons with energies from the mid-IR to THz regime will be very useful for mode-selective pump-probe experiments, which can be important for ultrafast “control” of these highly correlated systems.

Currently, most of the TR-ARPES were performed using table-top Laser system, which limits the choice of excitation photon energy that is important for performing APRES measurements on
wide variety of different materials. Therefore, it is important to have a tunable light source for TR-ARPES. On the other hand, the robustness of the APRES spectrum is limited by the space charging effect; thus, it is preferred to have ultrashort pulses with reasonable pulse intensity and reasonable repetition rate of the pulse. The actual pulse intensity and the repetition rate have to be determined for specific experiment.

**Photon-in/Photon-out spectroscopy**

For example: HR-RIXS, TR-RIXS, HR-XMCD, TR-XMCD, TR-Resonant Diffraction

Used for studying novel collective excitations of the electronic state (e.g. eta-mode of the superconducting state), selective excitations (CT and phonons) to study transient states and photo-induced phase transitions; superconductors (e-ph interactions, magnetism and superconductivity); magnetic materials (dynamics of the magnetic excitations); strong correlations in hard- and soft- condensed matter (charge transfer and phonon assisted excitations); and TR-magnetic X-ray diffraction Scattering for Vortex in SC (studying the magnetic vortex dynamics in SC and HTSC by pump (THZ)-probe (X-ray) techniques

**Ideal source for HR-RIXS:**

- Tunable photon energy in Soft X-ray regime (250 eV to 2 KeV)
- High repetition rate and beam stability.
- Narrow bandwidth of the monochromatic beam (Monochromator may be an option)
- Small beam spot on sample in sub-micron range: (1) sample in-homogeneous (2) domain physics (3) enhance detection efficiency without sacrifice resolution.

- Control of polarization.

Current sources limit Energy resolution of state-of-the-art RIXS in the soft x-ray regime at a level of the order of 100 meV (@ 1000 eV photon energy). This state-of-art RIXS machine is recently available in Swiss Light Source, which have revealed much lower energy excitations, such as spinon, magnon, and phonon in many of the transition metals oxides, first time seen using photons as a probe. To further revolve detailed behavior of these collective excitations and perhaps new-type of collective excitations posited at even lower energy, ultra-high resolution RIXS with a resolution of < 10 meV is ideal. Generally speaking, a light source with high repetition rate, narrow bandwidth, and small source spot is required to achieve ultra-high resolution for RIXS experiments.

**Ideal source for Time-Resolved soft x-ray RIXS (TR-RIXS)**

- Tunable Energy in Soft X-ray (250 eV to 2 keV)
- Requires very stable radiation sources
- control of the photon density per pulse
- control of the repetition rate (up to 10 MHz)
- control of the polarization
- FT limited pulses for the measurements in the time domain
- Tunable Pulse duration (sub fs to 100 fs)
- Tunable "pump" photon sources: in addition to the conventional optical pump, photons with energies from the mid-IR to THz regime will be very useful for mode-selective pump-probe experiments, which can be important for ultrafast "control" of these highly correlated systems.

Time-resolved pump-probe RIXS experiment can reveal much information about charge excitations when the system is driven out-of-equilibrium. To perform this type of experiment, it is required to utilities ultrafast x-ray pulse (< 100 fs) with sufficient intensity, which is just become available recently at the FEL facility. However, one has to be careful about the issues of radiation damage and spectrum distortion due to the intense pulse filed, which place the limit of the maximal pulse intensity for this type of experiment. As the damage threshold for each material is different, the optimal experimental condition has to be determined for each
individual case. Therefore, a light source with flexible choices of the pulse intensity and repetition rate is desired.

4.6 Mesoscale Material Dynamics

Most of this text is from a report of working groups led by Curt Bronkhorst, Joe Mang, and Don Hickmott of Los Alamos National Laboratory

Materials are central to every national need (i.e., security, energy, environment, transportation, energy security, etc.) and future technologies will place increasing demands on performance in a range of extreme conditions: stress, strain, temperature, pressure, chemical reactivity, photon or radiation flux, and electric or magnetic fields. To address the primary deficit in materials' understanding requires the means to find the operating physical mechanisms that occur in the microstructure. If these fundamental processes can be understood, exciting opportunities to use such extreme thermo-mechanical conditions to design and manufacture new classes of materials will open up.

The large deformation, damage and failure process for many polycrystalline metallic materials is inherently ductile in nature. In general, this means that the material will choose four specific physics mechanisms for accommodation of imposed deformation field or resistance to loading – solid-solid phase transformation, large deformation plasticity, shear localization or adiabatic shear banding, and cavitation. At present, materials models to represent this damage process contain the elements of pore initiation or nucleation, pore growth, pore coalescence, and ultimate failure. The nucleation process is believed to depend heavily on microstructural-based heterogeneities and the spatial distribution of defects. These include grain boundaries, impurity inclusions, intersection of twin planes, dislocation sub-cells. The statistical spatial distribution of inherent (grain boundaries, inclusions, initial dislocations) or deformation induced heterogeneities (twinning, dislocation subcell) is believed to act in combination with the spatial and temporal intensity of loading to determine which of the weakest defect sites will initiate a pore. A nucleated field of pores will then grow in size until they become large enough such that the deformation field surrounding individual pores begins to overlap with neighboring pores – at which time the process of damage coalescence begins. The coalescence phase is when the established pore field begins to join and when localization or adiabatic shear banding facilitates this process. Of course, ultimate failure will occur when the coalescence process brings about a percolated region of damage.

Dislocation cell structure in a deformed Cu sample (Cerrreta)
Successful addressing of this science will require the use of x-ray light sources to make 3D "orientation image" microstructure mapping to 1μm for the largest sample size, 3D chemistry mapping 1μm, and 3D initial dislocation/defect density mapping to 1nm for the smallest sample size. Samples range from multi-granular (10 grains or more) samples representative of bulk materials (100 microns – 1 millimeter in thickness) down to single-or-bi crystal samples of typically 10 micron size. The samples could be structural materials such as steel, minerals of importance to earth science, or energetic materials used for high explosives. Loading on the material could be done by a simple strain gauge (for low strain rates) up through laser drive at higher strain rates. There appears to be a very interesting regime between strain rates of $10^4$–$10^6$ sec$^{-1}$, where thermal activation transitions to phonon drag as a primary mechanism. Also, stresses in excess of 100 GPa up to 1 TPa appear to be of most interest for the frontiers of phase transition, EOS, and planetary science. Exceeding those strain rates at those stresses can place significant requirements on the brightness of an x-ray source for resolving strain of crystals or defect creation and dynamics.

Such experiments cannot be done now because:

- Very-hard x-ray sources are needed to penetrate the multi-granular samples.
- Repetition rates of at least 100 to 200 times more frequent than the physical process are needed for 3D imaging, i.e., rates of $10^6$ to $10^8$ pulses/second with $10^{10}$ or more coherent photons.
- Those sources need to be very bright, with <1 psec gating time to “freeze” phase transformations under loading.
- As the longitudinal coherence determines the number of resolution elements needed for imaging, a monochromaticity of order 1 nm/10 microns=$10^{-4}$ or better is required.
- The large spot sizes and higher x-ray energies for penetration imply very small diffraction speckle size, and either or both large distances to detectors and small pixels.
- Combining the high stress and strain rate environments with the required high-quality light source has not been done.

A possible design point for such experiments would use spot sizes of 50-100 micron at energies between 25–50 keV from an XFEL with good monochromaticity and excellent transverse coherence. Obtaining lasing at such high energies with significant brightness to get data requires emittance control; maintaining transverse coherence over such large beams may also be a challenge.

This drives the photon needs for mesoscale material dynamics:

- Hard X-rays: $>$20keV 100s of keV (penetration!)
- In some cases very high energy X-rays (to Uranium k-edge at 115 keV)
- "We need a hard X-ray flame thrower" (thanks Lou!)
- "Short pulses" on ~ps scales (ps phenomena at these length scales)
- Rep rate from single shot to kHz (e.g.: mapping strain deformations)

- For coherent imaging techniques
  - Monochromaticity of better than $10^{-4}$ (large field-of-view at high resolution)
  - Good transverse coherence length
- For inelastic X-ray scattering:
  - High spectral monochromaticity $<$10$^{-7}$ (energy resolution), high flux
4.7 Matter in Extreme Conditions – novel states of materials
Damage formation and propagation in radiation activated materials

For both fission and fusion, material response to activating radiation begins at the atomic level and evolves into larger-scale structural damage and deformation. The may portend a time-domain spectroscopic signal for defect formation and propagation on the femtosecond time-scale. This is fundamentally a hierarchical issue; at which length scale does an activating reaction trigger permanent large scale damage? Oxides of high-Z atoms, the primary fuel candidates for next generation fission reactors, may allow for a soft x-ray handle on this time domain question. A time resolved spectral technique in the soft x-ray regime could then study the initiation of damage formed by activated materials. We may not need high spatial resolution for such processes since here we only hope to energetically resolve the fast, atomic scale dynamics. Such an experiment might use an activating pump-probe with a subsequent soft x-ray pulse. It is the time resolved probe spectroscopy that will tell us about the trigger event in damage formation at the molecular level.

Alternatively, direct imaging methods, such as ghost imaging, could pick up what a soft x-ray study leaves off. Ghost imaging comes from the quantum entanglement of two photons produced by spontaneous parametric down conversion of an x-ray beam. In this case, the x-ray pairs are generated at a single atomic site. We then detect one photon in a non-spatially resolving "bucket" detector, and the other photon is collected in an array detector. Photons are only accepted in coincidence and so will likely benefit from time resolved synchrotron-like repetition rates, i.e. quasi-CW. The sample is placed in the beam destined for the bucket detector, potentially the very short wavelength partner. The longer wavelength partner, which might be below the absorption edge of the material, misses the sample and is collected in the array detector. The resulting long wavelength image then develops with the spatial resolution of the short wavelength partner. Such quantum-optical techniques for imaging the structural changes of activated materials might proceed in high density and high electron-temperature samples by passing >50keV photons through the sample while imaging the <20keV photon partners.

A more traditional approach would be small-angle x-ray scattering. In the 50-100keV regime, we can activate and then image many of the high-Z materials of interest to the nuclear energy program. Coherent x-ray diffraction could be used to image deformation fields inside in individual grains of the poly-crystal. While it would be very difficult to acquire a data set that would allow the full 3D deformation field to be recovered at 100ps time resolution, the evolution of the field projected onto a 2D plane may be feasible.

Time-scales of void formation and damage propagation.
Lab based Cosmic Spectroscopies

Numerous violent events that occur in our dynamic cosmos not only spark the imagination, but also pose some very interesting science questions. For instance, astrophysical x-ray sources such as accretion disks around neutron stars, black holes, and active galactic nuclei (AGNs) may reveal the origins of chemical elements or even the evolution of the Universe. Events like supernovae, hyper-novae, and gamma ray bursts (GRBs) are currently being addressed by space-based x-ray observatories: How do relativistic jets of matter form from accretion disks around compact objects? What type of events produces GRBs? What were the properties and life-cycles of the first, super-massive, stars?

The production of heavy elements is at the heart of this study. Elements and isotopes heavier than iron are made by neutron capture; half by a rapid-process and half by a slow-process mechanism. One open question is, where and when did the rapid-process neutron capture mechanism fill in the bottom half of the periodic table? Multiply charged iron ions are primary contributors to astrophysical spectra. Unfortunately, such spectra almost completely depend on atomic structure calculations which are known to fall short of the prize. Accurate lab measurements would therefore benchmark various theoretical approaches. One such class of experiments could be time-domain soft x-ray laser measurement of fluorescence rates. Typical experiments might involve (1) soft x-ray laser induced fluorescence on a relativistic ion beam or (2) pump/probe experiments that could access the fsec to nsec time scale with slow ions. The probe could be either a second soft x-ray pulse or an optical/UV pulse. Standard detectors can then directly provide time resolution for processes slower than a nanosecond.

Shock driven systems

In the mesoscopic limit, a sample may be shocked with a pulsed energy source and probed by hard x-ray scattering. Both direct imaging and diffractive imaging would reveal crucial information about transient phase changes, shock dynamics, and void nucleation/growth. As an example, phase contrast microscopy (PCM) splits an x-ray pulse into an object and reference pulses and reveals a probe-delay dependent interference pattern of the shocked sample. Transverse and longitudinal coherence are vital for such work. Covering the broadest range of targets would require hard x-rays while the single-shot nature of the experiment requires the highest possible x-ray pulse energy. In this case, high repetition rate is not so important.

We could also use such a technique to investigate shock induced defects in high pressure systems. Current theory cannot accurately predict the dynamics of shock-induced aerogel compression. Compression likely starts at a nucleation center and then propagates into structural failure. Again, since each event is random, we must obtain the imaging from a single pulse rather than stroboscopically from a sequence of identical events.
In the case of thin films, energetic optical lasers can deliver enough energy to the electrons in the target to drive a charge imbalance in the film. This breaks the quasi-neutrality and initiates an acceleration and compression of the ions. Bragg diffraction or phase-contrast microscopy with a bright hard x-ray pulse could reveal the time history of the ion motion while soft x-ray surface XPS of the shocked sample could reveal core electronic structure as the shocked film evolves.

In the case of nano-scale clusters, ultra-strong optical laser pulses can field-ionize a significant fraction of the electrons in a cluster. The collisional heating results in highly charged cluster plasmas with electron temperatures of 10eV - 1000eV. Such cluster plasmas are compatible with electron and ion time-of-flight spectroscopy whereby photo- and Auger electron spectra reveal the electronic conditions within the cluster as it ultimately disassembles by Coulombic or hydrodynamic forces.

**Photon needs:**

Further development of high energy density studies will require the following X-ray source properties:

1. Mesoscale studies (picosecond to nanosecond timescales)
   - Photon energies between 20-80 keV
   - ~1 picosecond pulses.
   - High intensity for single-shot measurements
   - Sufficient single-pulse intensity for single-shot measurements
   - Monochromatic; transverse and longitudinal coherence
   - High pulse-to-pulse stability
   - Synchronization of external drivers to X-ray pulses
   - Certain techniques (IXS and nuclear scattering) require high monochromaticity: ~1e-7 and less.
   - Development of highly monochromatic sources for higher efficiency.
   - Very small beam size, stability of beam (micron stability)
   - Two time regimes
     - Atoms: femtosecond time scales (XP-XP to within fs)
     - Mesoscale dynamics: picosecond to nanosecond time scales

2. Studies of atomic dynamics:
   - Photon energies between 8-20keV
   - 1 – 100 femtosecond pulses
   - Sufficient single-pulse intensity for single-shot measurements
   - High pulse-to-pulse stability
   - Synchronization of external drivers to X-ray pulses
   - Certain techniques (IXS and nuclear scattering) require high monochromaticity: ~1e-7 and less.
   - Development of highly monochromatic sources for higher efficiency.
   - Very small beam size, stability of beam (micron stability)

Single-shot measurements on shocked material experiments at the APS are currently limited in the atomic number (weight) of the materials that can be studied. This is essentially a penetration issue with the wavelengths available at e.g.: the APS. Meanwhile mesoscale measurements require a completely different type of source: crack propagation through diffractive imaging, can be at different length scales and higher energies. Picosecond time scales.
4.8 Biological studies at for Future Light Sources

Thomas Earnest

Biology is fundamentally dynamic, taking place over a wide range of spatial and temporal scales. Modern biological research increasingly focuses on the study of complex biological systems. Understanding the organized complexity and dynamics of biological systems requires the development of advanced tools and resources including a wide range of approaches from synthetic biology though light sources and computational tools. Synchrotron radiation has played an extremely important role over the past decades as a critical tool for investigating the structure and function of biological systems through the use of a number of techniques including x-ray crystallography, spectroscopy, and imaging. The initial generation of free electron lasers that have recently come into operation and other new light sources in the planning and development stages (including x-ray FELs and energy recovery linacs), have the potential to be equally as important and revolutionary, particularly for the study of biological dynamics. The potential impact of these sources in biological sciences involves the utilization of their coherence and the time structure. In this regard FELs, ERLs, and storage rings all have important and complementary advantages as no single technique can answer all the critical challenges of modern biology research.

The fundamental quantum of biology is the cell, where molecular and cellular events are tightly coupled in space and time. The ability to dynamically image cellular events at 1-5 nanometer resolution and with temporal resolution covering a range of interest in biology (femtosecond to second range) particularly when combined with atomic resolution information from crystallography or other methods, would revolutionize our understanding of complex biological systems. Furthermore time-resolved spectroscopic studies of biological molecules would enhance our understanding of their molecular function.

Future light sources, in concert with complementary approaches in molecular biology, synthetic biology, and biochemistry can enable the transition from measurement to control. For example many microbial systems have fully sequenced genomes and a broad range of molecular biological tools that allow for directed mutations and alterations of the genes (and subsequently the proteins that are their products). Time-resolved imaging of these cells combined with systematic perturbations in the component protein systems, particularly when viewed in the context of the genetic control circuitry of the cell, can allow for the determination of the roles of these components in cellular structure, function, and dynamics. These studies will require light sources spanning a wide range of beam parameters. Among these are high spatial and temporal coherence, high peak and average brightness, and pulses shorter than the phenomena of interest. Also critical is the flexibility of delivery of these pulses. This latter parameter requires a source of high intrinsic repetition rate such that the pulse structure can be delivered to best meet the need of a wide range of experiments. For instance the high resolution imaging of cellular structure to follow the dynamic localization of biological assemblies in the cell requires synchronization of the pulses with cellular events and the variation of the delivery of the pulses to interrogate the structure and function at numerous time points. Also this can assist in bunching pulses into microbunches that increase the flux onto the sample within the time-resolution limit of the phenomena being studied.

With these new tools covering a wide range of beam parameters, the fundamental basis of cellular signaling, photosynthesis, and multi-cellular phenomena can be investigated and this information can be utilized to the benefit of a wide range of problems in health, energy, and the environment. Further studies on the role of water in biology and of biomolecular self-assembly can improve our understanding of biology and serve as the basis for future technological advances.

Photon needs:
One clear result is that biological studies use and require a range of complementary analysis techniques, which in turn require access to a wide range of complementary X-ray sources ranging from water window (300eV) to whole animal imaging at hard X-rays (50 keV).

**Coherent imaging:**
- high rep rate, high brightness
- Full transverse coherence
- transform limited temporal coherence bandwidth
- Short pulses (down to 10fs diffract-destroy): LCLS++
- More photons
- CW, or quasi-CW ps pulses (static microscopy)

**Full field microscopy**
- Bright, incoherent source for full field microscopy, CW, narrow bandwidth, <2keV

**IXS, nuclear resonant scattering need**
- Highly monochromatic 1e-7 and less
- More flux!
- Flexibility of pulse trains, high rep rate
- Synchronization of triggers (photons) with pulses

To these ends we envisage that X-FELs, ERLs, and storage ring based systems will play important and complementary roles:

**X-FEL sources:**
- structure and dynamics of biological assemblies, cells, and multi-cellular organization;
- time-resolved biochemistry,
- fluctuation solution x-ray scattering; biological water

**ERL**
- coherent imaging of cells in three-dimensions;
- microcrystallography

**Storage rings**
- static crystallography;
- Laue crystallography;
- steady-state spectroscopy and solution scattering.

## 5 Desired properties of future X-ray light sources

The goal of this workshop is to identify the key photon source parameters required to enable breakthrough science across a range of different science interest areas irrespective of what type of facility may be required to deliver those photons. Studying the ‘dream photon source’ requirements for each of the science areas discussed above, we have identified the following classes of X-ray source as most likely to deliver groundbreaking new science not achievable with current X-ray sources:

1. **Ultra-short pulse, high peak power X-ray source**

Studies of the time-resolved dynamics of electrons and atoms require very short pulses (100as – 10fs – 100fs) in order to resolve atomic transitions and generate ‘snapshots’ of materials and chemical reactions as they occur. X-ray wavelengths must be tunable across atomic resonances,
and at least in the range from 1 keV to 12 keV to resolve spatial scales from nanometers to atomic resolution. Transverse and longitudinal coherence is required for most analytical techniques, as well as the ability to customize X-ray pulse duration and repetition rate on an experiment-by-experiment basis.

- Attosecond to 10s of fs pulse lengths,
- 200 eV - 15 keV photon energy range
- Sufficient coherent power for single-shot measurements
- Programmable pulse trains, pulse shaping, ability to serve multiple users
- Synchronization with fs pump lasers

Such a source would deliver breakthrough science in our understanding of chemical molecular dynamics, enabling the exploration and tailoring of reaction processes. It would enable new science in the study of time evolution of matter and facilitate the study of biochemical reactions and complex chemical interactions essential for the life and health sciences.

2. Picosecond, high peak power very hard X-ray source

Time resolved studies in mesoscale dynamics cover micron to mm length scales and would benefit greatly from a pulsed harder X-ray source that would enable time resolved studies on bulk materials. Picosecond X-ray pulses are adequate due to the larger length scales involved, however the X-ray energy regime should cover at least 30 – 100 keV, and possibly up to 150 keV for certain experiments. Monochromaticity and both transverse and longitudinal coherence are required for most analytical techniques, as well as the ability to customize X-ray pulse duration and repetition rate on an experiment-by-experiment basis.

- 30 - 50 - 150 keV
- Picosecond pulses
- Monochromatic
- Transverse and longitudinal coherence
- Synchronization with drive pulses for dynamic studies

Such a source would deliver breakthrough science in our understanding of time evolution of materials under dynamic loading, enhancing our understanding of material failure and enabling the engineering of novel materials based on a ground-up understanding of how materials behave under dynamic loading. Such a source also benefits the study of high energy density systems, advancing our understanding of materials under extreme conditions.

3. High-flux, high-brightness quasi-CW X-ray source

Spectroscopies demand high monochromaticity and benefit from the stability and narrow bandwidth offered by CW or quasi-CW light sources X-ray wavelengths must be tunable across atomic resonances, and at least in the range from 1 keV to 12 keV to cover interesting atomic resonances and resolve spatial scales from nanometers to atomic resolution in X-ray scattering experiments.

- 200 eV - 15 keV range
- Bright, high average flux, monochromatic, coherent, tunable
- Ability to serve multiple users

Such a source would advance the study of biological systems through permitting higher-throughput biochemical studies and microscopy on whole cellular structures. In addition, spectroscopic techniques employed by material scientists would benefit from the stability and narrow bandwidth offered by CW or quasi-CW light sources. Basically any technique that requires a monochromator immediately derives benefit from a stable narrow band source, whilst the increased flux speeds up data acquisition.
With these broad classes of X-ray source defined, it is now relatively straightforward to map these requirements onto the phase-space diagrams contained in the "Science and Technology of future light sources" white paper from December 2008. It should be noted that we specifically do not want to select any one technology over another – the goal of this working group was to define photon source requirements and then leave decisions as to the best technologies up to light source designers. However, one notable gap in technology is the very hard X-ray picosecond pulsed source – perhaps this gap can be filled with a non-lasing Linac solution such as SPPS but operating at higher energies?

Finally, the working group acknowledges that technological limitations may make it hard to design a ‘one size fits all’ photon source capable of satisfying all needs. Even covering portions of the photon parameter will deliver new science, and there remains space for both soft and hard X-ray FEL sources to co-exist covering separate parts of the photon energy regime in two or more separate facilities.

Mapping of the light source requirements onto the phase-space diagrams contained in the "Science and Technology of Future Light Sources' white paper from December 2008. One notable gap in technology is the very hard X-ray picosecond pulsed source regime required for mesoscale materials studies.

6 Summary

The “Science needs for new X-ray sources” working group at the 48th ICFA Advanced Beam Dynamics Workshop on Future Light Sources was charged with identifying the photon source
properties required to deliver breakthrough science beyond what can be achieved using currently existing X-ray light sources (including sources currently under construction). Participants identified a range of scientific research areas that would benefit from breakthroughs in light source technology, identifying the first experiments in a range of disciplines, and from this determined the photon source properties required to deliver new science. We therefore focused on the science areas, identified key first experiments in each area, and then looked for commonality in light source properties across different science areas.

A common theme from the workshop is that the next frontier in breakthrough science will be achieved by a transition from static studies to time-resolved studies of material behavior, chemical reactions and biology. Complex time resolved studies need sources with pulses on demand and time sequences tailored to individual experiments, and this is difficult to do at current storage ring based sources.

It is clear that no one new light source facility can serve the needs of breakthrough science in all areas. However across a range of science applications we found that there was a strong need for the following three broad classes of new light source:

1. **Ultra-short pulse, high peak power X-ray source**
   - Attosecond to 10s of fs pulse lengths,
   - 200 eV - 15 keV photon energy range
   - Sufficient coherent power for single-shot measurements
   - Programmable pulse trains, pulse shaping, ability to serve multiple users
   - Synchronization with fs pump lasers

2. **Picosecond, high peak power very hard X-ray source**
   - 30 - 50 - 150 keV
   - Picosecond pulses
   - Monochromatic
   - Transverse and longitudinal coherence
   - Synchronization with drive pulses for dynamic studies

3. **High-flux, high-brightness quasi-CW X-ray source**
   - 200 eV - 15 keV range
   - Bright, high average flux, monochromatic, coherent, tunable
   - Ability to serve multiple users

As with any summary, this information taken in isolation is dangerous and should be read in context of the entire working group report!