

Beamline for *in situ* studies of chemical transformations by combined, synchronous and “quick” x-ray absorption and scattering measurements (QAS)

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A. Science Case

The QAS beamline is proposed as part of the suite of beamlines (see Appendix A) for Chemical and Energy Sciences (CES). The CES community includes scientists from academia, national laboratories and industry who work in catalysis, electrochemistry and energy conversion/storage fields. The key scientific drivers these groups share are: the atomistic real-time understanding of the mechanism of chemical reactions and catalyst deactivation, the design of new or more efficient chemical processes, the more efficient design of high-activity, high-selectivity, and low-cost catalysts, development of renewable energy conversion technologies, storage of energy products, and portable devices for energy delivery. The main scientific challenges in these closely related sciences are outlined in the Appendix A. It is the goal of this proposal to overcome the present inability to study multiple scales of spatial and temporal metrics *in situ* and *in operando*, and measure fast kinetics (faster than with 1s time resolution) of working catalysts. Among the multiple scales of spatial and temporal metrics we mention typical dimensions characterizing atomic bonds: 0.2 nm, nanoparticle catalysts: sub-nm to nm, support materials: nm- μ m, reactor compartments: mm to cm. The practical time scale of most chemical reactions ranges from 0.1ms to s, nucleation and growth rates from s to min, reaction rates s to h, and catalyst degradation rates from minutes to days to months. QAS beamline will be used for studies of the large class of model nanoscale systems undergoing real-time chemical and physical transformations, including those with characteristic times of the order of 100 ms or less. Due to the large demand for high time resolution experiments in CES and environmental sciences where the real catalytic systems, dilute soil and water contaminants, low dimensional electronic devices, have to be studied *in situ* and *operando*, a dedicated, high-flux beamline (TRS) is also proposed that will be optimized specifically for high time resolution experiments with dilute or low dimensional materials.

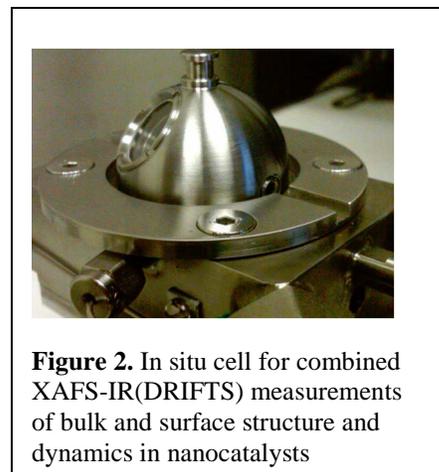
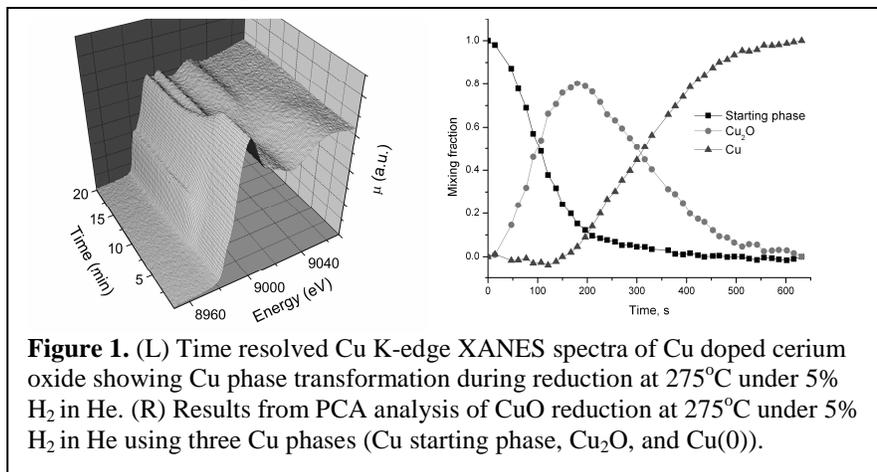
The planned *in situ* investigations will significantly impact CES research because they allow to investigate the mechanisms of chemical reactions and their dependence on the complex, dynamic interactions of

reactants and products with both nanocatalysts and their support. Although there is a number of beamlines in the European synchrotrons that combine techniques for studying gas-solid interactions (e.g., XRD and IR, Quick scanning EXAFS and IR), the proposed beamline will be the first in its class due to: 1) the capability to run combined, synchronous measurements of XAFS, XRD, Diffraction Anomalous Fine Structure (DAFS), Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) with the analysis of the gas phase by Mass Spectrometry (MS), and 2) the specially designed infrastructures for *in situ* research in a number of closely related fields in chemical engineering, environmental science and materials science. As described in the Table I of the Appendix A, there is strong synergy between the science done at the QAS beamline and the other beamlines of the suite (XANES, high-energy X-ray diffraction/PDF, XPS/NEXAFS). Together, these beamlines will help solve a complex problem of multiple scales that are intrinsic to the spatial and temporal metrics of the structure and dynamics of catalytic systems.¹ The aim is to supply the users with the world-best experimental possibilities for measuring *in situ* physicochemical processes in a broad range of materials using multiple complementary techniques, including those that can be done with 10ms time resolution. This requires an excellent performance of the beamline making optimal use of NSLS-II source, state of the art QEXAFS monochromator, specialized infrastructure for *in situ* experiments, appropriate sample preparation facilities and experienced staff for user support. This facility will open up new possibilities for academic and industrial sciences.

The new scientific opportunities available at the QAS beamline include the following examples:

I. Investigations of structure, kinetics, dynamics and reactivity during the in situ transformations with down to 10 ms time resolution

Chemical transformations: Studies of chemical reactions in real time with sub-second time resolutions offer many rewards in catalysis science (since many reaction turnover rates are of the order of a few seconds or less) and are very challenging experimentally. The best time resolution needed in the studies of homo- and heterogenous catalysis is diffusion limited to ca. 10 ms. Until the invention of Quick scanning Extended X-ray Absorption Fine-Structure (QEXAFS) technique,² most alternatives to the real time approach were various *ex situ* methods of physical or chemical trapping of reaction intermediates with the side effect of altering reaction pathways which are temperature-dependent. The first in US dedicated QEXAFS facility was developed by scientists from NSLS, BNL-Chemistry, as well as Yeshiva University, University of Delaware and Lehigh University, and is now available for users of Synchrotron Catalysis Consortium.³



This instrument allows the acquisition of time-resolved data in a variety of systems relevant to electrochemical, photochemical, catalytic, materials and environmental sciences (Fig. 1). At the QAS, projected time resolution will be improved to 10 ms, as we intend to use an optimized version of the QEXAFS monochromator used at the SuperXAS beamline at the Swiss Light Source. In addition to analyzing reaction product online using mass spectrometry (MS) synchronously with the XAFS measurements we will measure catalyst-adsorbate interactions in real time with XAFS using DRIFTS

technique, the combination pioneered by M. Newton (ESRF). SCC members (N. Marinkovic, Q. Wang and A. Frenkel have built and successfully tested a dedicated instrument (Fig. 2) for combined XAFS/DRIFTS/MS measurements. It will be ready for use at the NSLS-II.

Glass transition, nucleation and crystallization studies: In view of the engineering challenges identified by National Academy of Engineering, glass will remain a key high-tech material to solve major problems of various technologies, provided we can understand correlations between glass-forming ability, compositional trends of physical properties and glass structure. Novel products, like self cleaning, heat absorbing and intelligent, switching glasses form a growing market based on embedded nanoparticles. Understanding of atomic dynamics during heating/cooling (quenching) of glass-forming systems remains a key challenge of condensed matter physics and applications of glass. The glass transition is still not well-understood from an atomistic point of view. Numerous theories are proposed and a large number of researchers are actively studying this problem,⁴ but the real atomic/molecular dynamics associated with liquid to glass transition and relaxation are not well understood to date. Experimental verification of theoretical predictions is difficult, because of the lack of suitable techniques capable to follow the temperature-driven structural changes at the nanoscale. The recent development of QEXAFS technique at X18B beamline at NSLS has made possible the observation of the temperature-driven changes in the short-range structure of network glasses using linear temperature ramp as in differential scanning calorimetry (DSC) experiments. Preliminary heating experiments performed by the Lehigh research group demonstrated atomic dynamics at glass transition to be essentially cooperative in nature, which can be identified by QEXAFS when the glass satisfies some specific criteria. Glass community will utilize the QAS beamline for temperature dependent, simultaneous QEXAFS/XRD/IR measurements in order to establish changes in molecular structure of glasses. So far researchers have been able to probe the region only around T_g (α -relaxation). With 10-ms QEXAFS, they can make the measurements in \sim ms time range, and begin probing the origin of β -relaxations as well (Fig. 3). Nucleation and growth of nanocrystals in glasses are at the heart of the synthesis of glass ceramics for various technological application ranging from non-volatile optical memory devices to bioactive implants. An understanding of the dynamics of the short-range structural changes associated with the ceramming process plays a key role in controlling the physical properties of the resulting glass-ceramics where *in situ* time-resolved QEXAFS spectroscopy at high temperature may become the technique of choice for studying such phenomena at atomic scale.

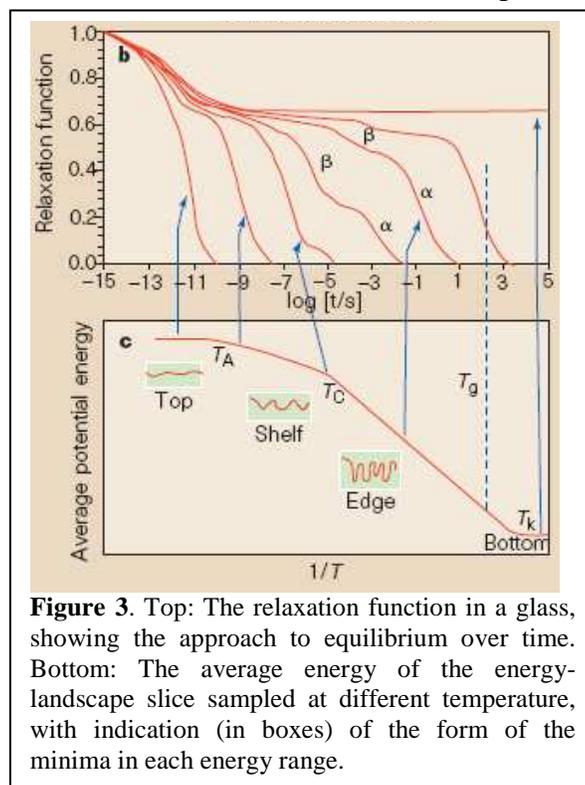


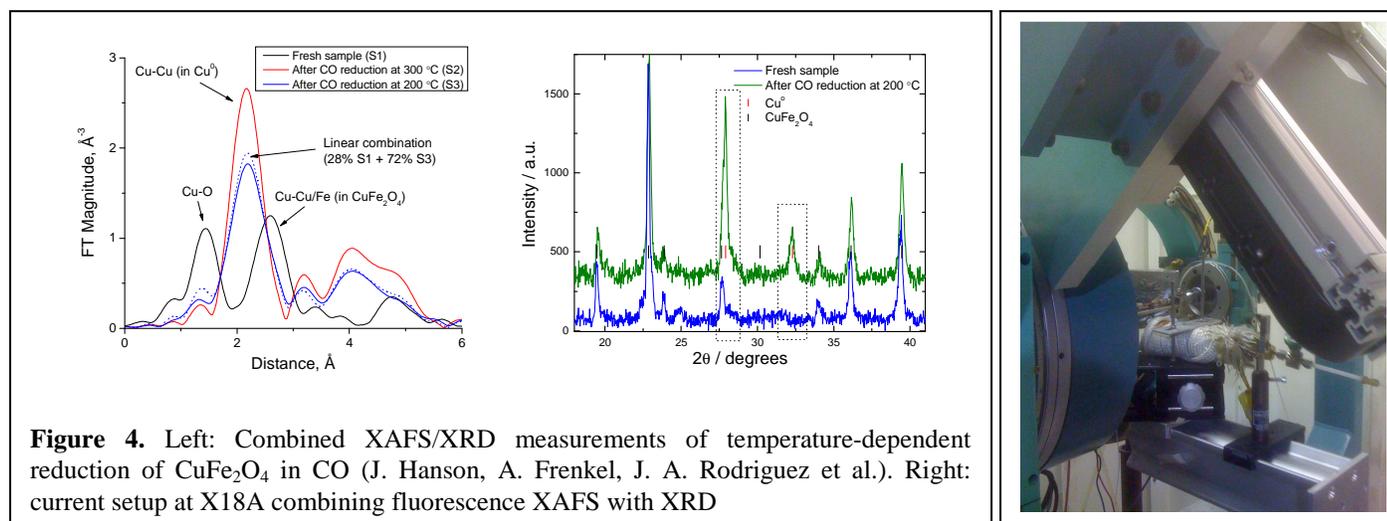
Figure 3. Top: The relaxation function in a glass, showing the approach to equilibrium over time. Bottom: The average energy of the energy-landscape slice sampled at different temperature, with indication (in boxes) of the form of the minima in each energy range.

Environmental Science: Members of the research group of Prof. Donald Sparks (U. Delaware) have conducted studies on the kinetics of rapid chemical processes on mineral surfaces and soils, e.g., sorption, redox and precipitation reactions. Since many of these chemical processes occur on very short time scales (seconds and minutes), spectroscopic techniques with fast data acquisition time like QEXAFS, in which one can follow the kinetics of rapid reactions at the molecular level, are the ultimate way to study reaction mechanisms at environmental interfaces. Additionally, QEXAFS is particularly useful for environmental applications because it is an *in situ* technique and thus one does not need to alter natural samples, by drying or placing under high vacuum. The ability to capture rapid reaction processes involving sorption, redox, and precipitation phenomena is important since in many cases, a large part of the reaction processes are completed before measurements can be made using traditional batch and flow techniques. Consequently,

our new possibilities enable to gain important mechanistic information and to verify the correct model for the chemical kinetic parameters.

II. In situ studies of real catalysts by combined absorption and scattering techniques

Chemical transformations: XAFS and XRD techniques provide complementary information about the structure of catalytic materials: XRD is effective in pure or mixed crystalline materials while XAFS provides short range order structural features in less ordered, nanosized or amorphous materials. In addition, XAFS also gives element specific information about the electronic properties of the element being probed at its absorption energy. Finally, the DAFS technique discussed in greater detail below allows the assessment of the local structure in ordered species within heterogeneous samples, for those systems in which ensemble-averaged XAFS data analysis would be complicated by different forms of the resonant element. These three methods have been developed and advanced *independently* from each other at synchrotron sources in the US and abroad. To analyze catalysts under their operating conditions, a new approach that allows the simultaneous collection of the XRD and XAFS data under *in situ* conditions together with online product analysis is required. At present, XAFS and XRD measurements can be performed at the NSLS only at separate beamlines, with acquisition times of $1-10^3$ s for XAFS and $10-10^2$ s for XRD. DAFS has been performed only a few times in the last 10 years, and has been used rarely in catalysis and hydrogen storage applications, for which it would uncover otherwise inaccessible details of their heterogeneity. The members of the SCC and NSLS teams are currently building the first in the US instrument dedicated for combined, time-resolved Quick XAFS/XRD experiments at beamline X18A of NSLS. It will be the prototype



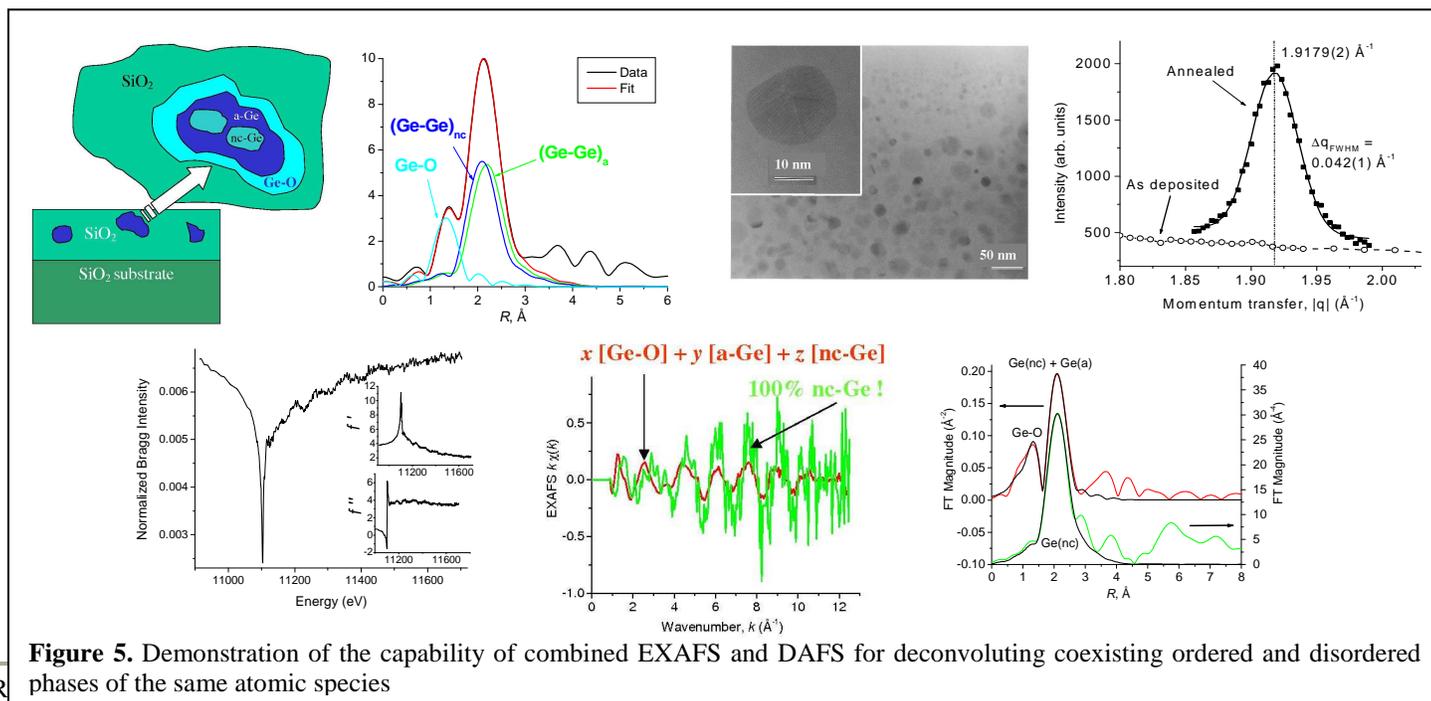
instrument for the QAS beamline. Such a combination will allow the measurement of changes in the actual structure (in the short, medium and long range order), electronic properties and chemical activity of heterogeneous catalysts simultaneously. This will be coupled with online gas analysis, dedicated for studying *in situ* chemical transformations. The current setup includes transmission and fluorescence XAFS chambers, position-sensitive linear detector (INEL) as well as a Perkin-Elmer amorphous silicon 2D detector and residual gas analyzer (mass spectrometer), along with the automated gas mixing system. Fig. 4 shows results of the first successful test of this new instrument. CuFe_2O_4 is a well known precursor for copper catalysts with high thermal stability and activity. It is used as a catalyst in hydrogen production, thermal decomposition of ammonium perchlorate, and is potentially useful in water-gas shift reaction. Its structural transformation upon reduction cannot be fully understood by XRD technique alone, due to the likelihood of forming metastable, short living, strongly dispersed, and/or disordered phases toward formation of pure Cu. Such phases will be invisible to diffraction, which is a long range technique, but will be detectable by XAFS which, in turn, allows to get short range structural information. In addition, absorption spectroscopy yields invaluable information about the chemical valence of the absorbing atoms. Only by combining these techniques in one experiment, where the sample is subjected to the same

temperature/gas treatment conditions one can detect both the short range and the long range structure of this system *in situ*. Fig. 4 (left) shows Fourier transform magnitudes of EXAFS data, demonstrating that the sample reduced at 200 °C and cooled down to room temperature is a linear combination of the fresh sample and the fully reduced sample. XRD data obtained in the same sample (Fig. 4, right) shows presence of the same two phases as well, enabling the possibility of the self-consistent interpretation of these two techniques. This instrument, as well as the knowhow that we are acquiring will be used at the QAS beamline of the NSLS-II.

Electrical energy storage: Batteries are complex and dynamic devices that rely on a series of intricate mechanisms, involving ion transport, charge compensation, structural changes, the formation of metastable phases and thermodynamic instabilities. The development of high capacity, safe lithium batteries requires new tools to better understand the physical and chemical processes that occur during cycling and the ability to predict and ultimately control the key electrochemical properties such as capacity (power and energy density), durability (calendar and cycle life), abuse tolerance (safety characteristics) and cost. XAFS and XRD are essential tools used in *in situ* investigations of charge compensation (oxidation/reduction of a transition metal) and structural transformations in working electrochemical cells. Changes in these fundamental material properties can be related to electrochemical properties, such as cell voltage, capacity, rate capability and capacity fade. Currently, XAFS and XRD data are acquired on separate beamlines and require medium-long acquisition times ($>10^3$ s). The capability of combined, time-resolved quick XAFS/XRD will allow us to see real time changes in the electrode structure and chemical bonding during electrochemical cycling. The fast acquisition times will give us the opportunity to investigate the electrode at greater current densities (rapid cycling rates), which is currently not feasible at NSLS beamlines.

III. Resolving the local structure in heterogeneous mixtures of ordered and disordered nano-phases

Diffraction Anomalous Fine Structure (DAFS) is a powerful technique that combines long range sensitivity of XRD and local structure sensitivity of XAFS.⁵ DAFS technique allows the determination of the local structure in each ordered species within heterogeneous samples, for those systems in which ensemble-averaged XAFS data analysis would be complicated by a coexistence of different physical forms of the resonant element. By combining EXAFS and DAFS it is possible to quantify each phase in a mixture.⁶ Such combination is particularly powerful when at least one phase is disordered and not amenable to XRD studies. DAFS has been never used for studies of heterogeneous or multi-site real catalytic or battery systems such as metal nanoparticles, metal oxides, and others. As the schematic (Figure 5, taken from Ref. 6) shows, a typical sample for such study (top left) would consist of a number of ordered and disordered phases – shown here using Ge-based phases as an example. EXAFS and electron microscopy data show



presence of three types of Ge: 1) ordered (nanocrystalline, average size 15 nm), 2) ordered (Ge oxide) and 3) disordered (amorphous Ge) phases. Selecting a Bragg peak corresponding to the nc-Ge, it is possible to obtain nano-DAFS signal on that peak and deconvolute EXAFS oscillations from the nc-Ge phase only. Combining with the EXAFS signal from the sample, the rest of the phases can be discriminated as well.

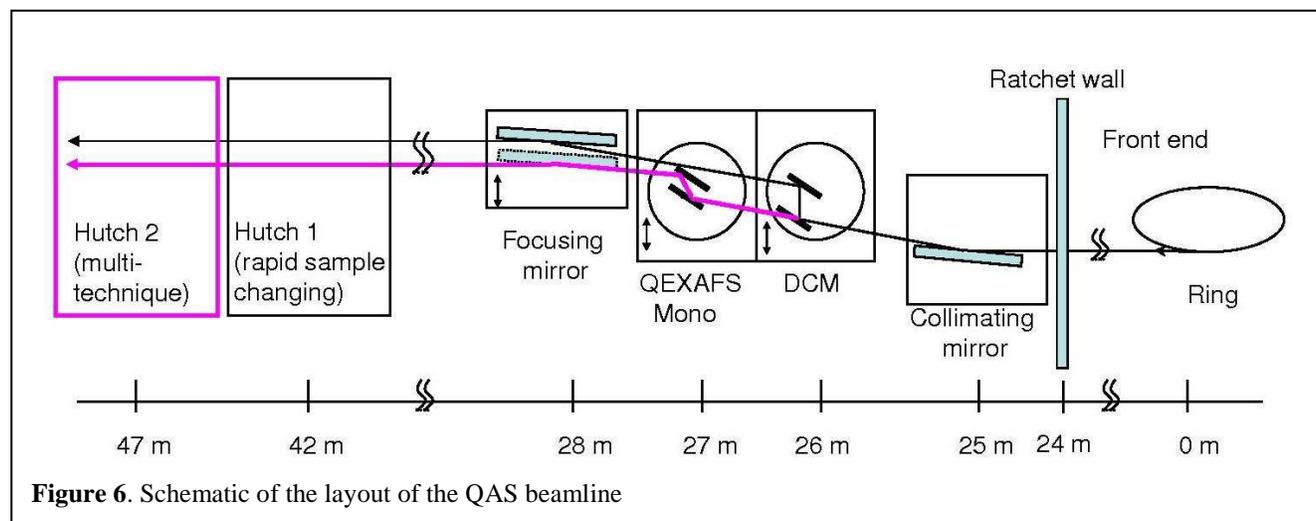
When these capabilities are enabled, different scientific communities (CES, glass community and the environmental science community) that join forces in proposing the QAS beamline will be able to perform:

- 1) in situ, time-resolved or potential-resolved studies of chemical transformations with coexistence of reactants, intermediates, and products. In catalysis science, such capability is needed for characterizing the structure of catalysts in heterogeneous reactor compartments. For the R&D of fuel cells, it will be used for studies of mechanism of the low temperature ionic conductivity (e.g. in $\text{SrMO}_{2.5+x}$, $M = \text{Co, Fe}$)
- 2) in situ studies of nanocatalyst activation (e.g., partially reduced metal oxides and fully reduced metal nanoparticles),
- 3) in situ studies of phase change materials (e.g., glasses or memory alloys) containing a mixture of ordered and disordered phases (see schematic).

B. Beamline Concept & Feasibility

The beamline source will be a 3-pole wiggler. The beamline optics will include (Fig. 6):

- 1) A collimating mirror, Rh coated, 1m long x 100 mm wide, water cooled, ~25 m from the source (2mrad, energy cutoff 34 keV). The energy range will be 4.5-34 keV.
- 2) A double-crystal (Si (111)), fixed-exit monochromator (~26 m from the source) with a stepping motor mechanism for combined, slow scanning XAFS and DAFS.
- 3) A double crystal, channel cut monochromator (~27 m from the source) with a cam-driven rotation mechanism (for in situ QEXAFS),
- 4) Toroidal focusing mirror ~ 28 m from the source; 2:1 focusing (horizontally and vertically).



There will be 2 endstations: the upstream endstation (37 m from the source) will be used for large area samples which can be rapidly replaced between experiments. Examples of such studies include reaction/oxidation reaction in concentrated catalysts investigated by time-resolved, temperature-resolved and/or QEXAFS. The downstream station (42 m from the source) will include setups for specialized cells and reactors such as: an oxidation/reduction cell for XAFS/MS, a capillary cell for QEXAFS/XRD/DAFS/MS, a clam shell furnace cell with rapid data collection for QEXAFS/MS, a cell for QEXAFS/DRIFTS/MS, in situ electrochemistry cell, in situ fuel cell, in situ battery cell, a laser irradiation facility coupled with QEXAFS sample cell for glass research, as well as other specialized cells used by the CES, glass and environmental science communities that require extensive alignment. Some pre-processing

and reactivity studies of the samples can be done in the second hutch while the first hutch is in use. We envision several setups, internally aligned, for most advanced complementary instruments.

Flux and time resolution: A 1m long collimated mirror (2mrad) will accept 2mm of the beam vertically, which corresponds to the 0.08 mrad vertical acceptance for the 25 m from the source. Horizontal spread of the beam at 25m, assuming 4 mrad horizontal divergence is 100 mm, i.e., entirely acceptable by a 100 mm wide collimating mirror. Fig. 7 shows calculated flux curves at the distances right after the monochromator and at the image plane of the focusing (2:1) mirror.⁷ This preliminary design was chosen to represent a realistic optical layout. It is expected that at the detailed design phase, several other possible optical designs, such as placing the first mirror inside the shield wall, will be considered and the best option will be chosen. Such a detailed effort is not appropriate at this stage of the proposal, however, we anticipate being able to achieve $\sim 1 \times 10^{12}$ photons at the sample. Such flux is approximately the same as the flux at the SuperXAS beamline at the SLS.⁸ We expect to reach a similar performance at QAS in terms of the time resolution (10ms) and signal to noise ratio as in this currently world-best QEXAFS beamline.⁹

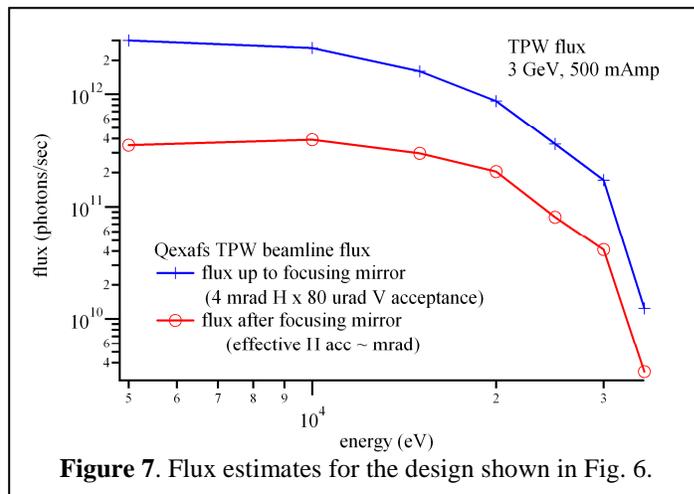


Figure 7. Flux estimates for the design shown in Fig. 6.

C. Required Technical Advances

There are several challenges that need to be resolved to reach the level of performance targeted for this beamline. For example, one challenge is the physical integration and alignment of reactor cell or DRIFTS cell with XRD XAFS and IR detectors, in a manner which allows for simultaneous measurements. Another challenge is the internal and external synchronization of the gas input system, which also has to facilitate very fast changes of the gas composition, temperature controllers and chemical analysis system with detectors and X-ray and IR sources. There is a need to develop and support a control system to operate these instruments, in a user-friendly manner. In QEXAFS experiments, 10 ms scan duration requires new detectors, fast ion chambers/photo diodes, and electronic amplifiers. SCC members together with NSLS staff and users have been developing such combinations at the beamlines X18B, X19A and X18A since 2005, and have acquired the experience in coordinated measurements with QEXAFS, XRD and reaction control and product detection. The tests are under way with DAFS, QEXAFS and IR. Integrated control systems currently under development for combined experiments at X18A will be used as a prototype of the new control system at the NSLS2 for this beamline.

D. User Community and Demands (The lists of scientific communities and potential user groups are in the Appendix C)

The synchrotron CES community consists of scientists using synchrotron radiation in the areas of chemical transformations, catalysis, electrochemistry, energy conversion/storage, and hydrogen storage research. While the QAS beamline will be a more advanced facility compared to the existing NSLS beamlines, the CES user community at the existing beamlines X18B, X19A and X18A can be used to sample the future interest to the proposed beamline. The CES community interested in the QAS beamline consists of currently ~ 59 groups from academia (35 – chemistry / 24–energy sciences), 19 from national laboratories (10/9), and 6 from industry (2/4). The total of 84 groups represents about 500 experienced synchrotron users (400/100). For the detailed list of the potential users of the QAS beamline see [Appendix C](#). The Synchrotron Catalysis Consortium (SCC) is a user organization created by initiative of scientists from academia, national laboratories and industry, and supported by a grant from DOE-BES. Members of SCC promote their synchrotron expertise to other CES members, involve them in synchrotron research by organizing

workshops, training courses and on-site personal training sessions, and develop strategic plans for transferring and expanding synchrotron CES research to NSLS2.

SCC members have attracted new users to the plans for the QAS beamline. Specifically, there is tremendous interest in the glass community (Appendix C), lead by the NSF's International Materials Institute (IMI) for New Functionality in Glass at Lehigh University (Director: Professor Himanshu Jain) to utilize QEXAFS capability at the QAS beamline. Members of the glass community are interested in glass formation from the melt, which is a time and temperature dependent phenomenon. Recently, they made some very fundamental observations regarding structural evolution only due to the time dependent EXAFS analysis made possible by QEXAFS at beamline X18B. The IMI group and their international collaborators have new programs on laser-induced crystallization of glass. They have succeeded in "writing" single crystal ferroelectric architecture in glass, and received a DOE grant for a new project to develop this area of material fabrication. Toward that goal they will need to study the glass to crystal formation under laser irradiation using QEXAFS. According to Prof. Jain, complementary spectroscopic (XAFS and IR) and XRD tools will be needed to understand the overall phenomena. A. Frenkel was one of the speakers at the first Glass research workshop held at BNL in 2009, following which the new ties between the leading PIs in the glass community and the CES were formed. As a result, Professor Jain expressed support for the QAS beamline proposal and offered help in reaching out to other members of glass community, in the US and abroad.

There is a growing environmental sciences community that is interested in following reaction processes in real time at the molecular scale. SCC is interested in joining forces with these groups, as we have been successfully collaborating in the past developing new applications (e.g., QEXAFS) and solving similar problems in data acquisition and analysis methodologies. Members of that community (see Appendix C) conduct studies on the kinetics of rapid chemical processes on mineral surfaces and soils, e.g., sorption, redox, and precipitation reactions. According to Prof. Sparks (U. Delaware), additional groups (from Stanford, LBNL, U. Kentucky, EPA, Cincinnati and ETH, Zurich) are expected to be interested in QEXAFS studies at the QAS beamline.

Five SCC members, NSLS scientists, the group of Dr. Sparks, and scientists from Lehigh University have jointly developed new expertise (and coauthored an article in RSI in 2010) in using QEXAFS for problems of their respective communities. They plan to transfer this knowhow and continue their collaboration at the QAS beamline at NSLS2.

User training

Optimal, efficient use of the proposed facility requires specialized training of the potential users, especially with respect to time resolved, in situ studies. In the past six years SCC members have been very active in organizing workshops and training courses for CES users, as well as for the larger community of EXAFS users. These workshops and training courses are run annually since 2005. In particular, the feedbacks on the training courses on EXAFS measurements and analysis have been overwhelmingly positive from well established, relatively new to the synchrotron, and potential future users from the catalysis community. As part of the proposed efforts we plan to combine and expand several existing venues, including annual training courses in EXAFS theory, analysis and applications to nanoscience and catalysis, catalysis workshop at the Annual NSLS/CFN Users Meeting and the web-based EXAFS training course, to provide more frequent training targeted to students and postdoctoral fellows from the catalysis and electrocatalysis research groups. Existing courses that SCC members organized were oversubscribed by at least two-fold. Travel funds are available to the attendees via the grant of the DOE to the SCC. As in the past, we will also support new research groups who need travel support. In continuation of the effort started six years ago, we will continue with the dissemination of major initiatives electronically, using our web site: <http://www.yu.edu/scc> and the recently created web-based forum for information exchange ([scc-forum]). These resources are used by experienced and new synchrotron users to get updated on the upgrades at the SCC, new training courses and workshops, as well as to ask a question about data analysis, instrument availability, or to get help in designing a new experiment.

E. Proposal Team Expertise and Experience (Curriculum Vitae of the team are in Appendix B).

Dr. Anatoly I. Frenkel is a Professor of Physics and Chair of the Division of Natural Sciences and Mathematics at Yeshiva University. His main research interests and expertise are in the areas of structure and properties of nanomaterials. He is a spokesperson of the Synchrotron Catalysis Consortium. Frenkel has 19 years synchrotron experience at the NSLS, APS and ESRF. Frenkel has published ~150 articles on the instrumentation, applications and data analysis methods in XAFS. He developed data analysis and modeling methods for monometallic and heterometallic nanocatalysts. These methods are now widely used by members of catalysis community. He is an organizer of many XAFS training courses, conferences and workshops in nanoscience and catalysis, at Brookhaven and elsewhere.

Dr. Simon R. Bare is a Senior Principal Scientist at UOP LLC, a Honeywell Company. His main interests are in understanding structure-function relationships in catalysts using primarily in situ characterization methods. He has over 20 years experience using synchrotron radiation-based techniques, primarily X-ray absorption spectroscopy, using beamlines at NSLS, APS, SSRL, HASYLAB and BESSY. He has published over 70 publications, and has presented many invited seminars nationally and internationally. He has collaborated with many groups worldwide, and is UOP's spokesperson for the SCC at NSLS and MRCAT at the APS. He is a member of the Light Sources Directorate SAC at BNL, and a member of BESAC. Drs. Bare and Frenkel are members of the Organizing Committee for the Operando-IV Congress, to be held in Brookhaven National Lab in 2012.

Dr. Jinguang G. Chen is the Claire D. LeClaire Professor of Chemical Engineering at the University of Delaware. He started his synchrotron research during his tenure at the Exxon Research and Engineering and was the Spokesperson of the Exxon U1A Beamline. His earlier work provided a unified methodology for NEXAFS studies of inorganic compounds; his review article ("NEXAFS Investigations of Transition Metal Oxides, Nitrides, Carbides, Sulfides and Other Interstitial Compounds", *Surface Science Reports*, 30 (1997) 1-152) remains to be one of highly cited references in NEXAFS research. In 2005 he and colleagues established the Synchrotron Catalysis Consortium (SCC) at the NSLS. SCC members have enhanced the synchrotron capabilities for catalytic applications and significantly improved access to synchrotron techniques by researchers from academic, industrial and national laboratories.

Dr. Steven Ehrlich is a physicist at the National Synchrotron Light Source at Brookhaven National Laboratory. He serves as User Liaison and Experimental Operations Manager of the NSLS. He coordinates operations with internal and external research groups and facility users, troubleshoots operational problems at beamlines, runs the weekly X-ray/VUV users meetings, and creates and distributes weekly X-ray/VUV users meeting minutes. He also provides NSLS experimental users an interface with machine operations and NSLS and BNL staff. He is the spokesperson for beamline X18A. He is in the process of completing an upgrade of the X18A beamline, part of which adds EXAFS and quick EXAFS capabilities to the scattering and diffraction line. He has worked with the Synchrotron Catalysis Consortium (SCC) to optimize beamline X18A for EXAFS, quick EXAFS and combined EXAFS/diffraction measurements. His research includes structural studies of long alkane films, noble gases confined in porous media and liquid systems.

Dr. Jason Graetz is a Materials Scientist at BNL. He is interested in ex situ and in situ synchrotron techniques to investigate microstructural, morphological and electronic structural changes occurring in energy storage materials during charge/discharge reactions. He has used XAS to study catalysts in reversible hydrides and measure charge compensation in lithium cathodes and XRD, SAXS and WAXS to determine the structures of new materials and study structural changes in lithium electrodes and metal hydrides during cycling. Dr Graetz is a U.S. Expert of the International Energy Agency on hydrogen storage. He was the recipient of the 2006 Ewald Wicke Award for his work in physical chemistry of metal hydrides and recently received the Presidential Early Career Award for Young Scientists and Engineers (PECASE).

Dr. Jonathan C. Hanson is a chemist whose main research interests are in the areas of catalysis and diffraction sciences. His research is supported by US-DOE. He is spokesperson for beamline X7B at the NSLS and has contributed to the development of combined XRD/QEXAFS at beam line X18A. He has

more than 18 years of experience working at synchrotrons, x-ray absorption spectroscopy and time-resolved x-ray powder diffraction in his studies. He has published over 210 articles.

Dr. Syed Khalid is a beamline scientist, spokesperson and research engineer of the facility beamlines X18B and X19A at NSLS for XAS. He has 30 years experience in synchrotron research and instrumentation, using SSRL, CHESS, Photon Factory (Japan), Alladin and NSLS. He built XAS equipment at the Department of Chemical Engineering, University of Delaware. He developed the EXAFS and QEXAFS instrumentation at beamline X18A and X18B. He helped developing the X9 beamline for biological EXAFS (now X3). He trained a few hundred users to operate X18B and X19A beamlines, resulting in a few hundred publications coming out of these two beamlines (average about 70 / year). Khalid also helped organizing and was a speaker and instructor in the annual XAFS workshops at NSLS. He has about 80 publications.

Dr. Jose A. Rodriguez is a chemist whose main research interests are in the areas of catalysis and surface sciences. He is spokesperson for beamline X7B and contact person for beamline U7A at the NSLS. He has more than 15 years of experience working at synchrotrons, using photoemission, x-ray absorption spectroscopy and time-resolved x-ray powder diffraction in his studies. He has published over 250 articles and has given many invited seminars about synchrotron-based techniques for catalyst characterization.

Dr. Xiao-Qing Yang is a material scientist and PI for the Applied Battery Research for Transportation (ABRT) and Batteries for Advanced Transportation Technologies (BATT) projects at BNL. The goals of these projects include synthesis and characterization of new cathode, anode, and electrolyte materials with improved calendar and cycling life, better abuse tolerance for lithium batteries. He has developed several new synchrotron based x-ray techniques for in situ characterization of battery materials. He was awarded several US patents. Dr. Yang organized and co-organized several international conferences, such as IBA2007 in Shenzhen and CIBF2006 in Beijing. He is one of the organizers and the general secretary for the 14th International meeting of Lithium Battery (14th IMLB) in Tianjin, China, June 22, 2008. Dr. Yang was elected as a member of the board of directors of the International Battery Materials Associate (IBA) in December of 2008.

F. Suggestions for BAT Membership

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