

International Workshop on Improving Data Quality and Quantity for XAFS Experiments (Q2XAFS 2011)

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An introductory overview to the special issue papers from the Q2XAFS Workshop in this issue of the journal.

X-ray absorption fine structure (XAFS) is now a well established method for characterization of local structures and electronic states of chemical species in materials, biological and environmental sciences. Moreover, the user base of XAFS has broadened so that it is no longer only practiced by specialists but also by researchers from a range of scientific disciplines. The first attempts at establishing standards for experimental practice and the quality of data and analysis were begun nearly 25 years ago and, as the field is now burgeoning, this is more important than ever. Thus, early reports on standards and recommendations appeared in 1992 and 2000, but significant updates have not been published since that time. Developments in beamline and detector technology, together with the establishment of third-generation synchrotron radiation sources, have enabled significantly improved XAFS quality and throughput, and allowed new and novel experiments previously not possible. Thus, new discussions of XAFS standards and criteria are particularly timely.

Q2XAFS (International Workshop on Improving Data Quality and Quantity for XAFS Experiments) was intended to establish new standards and criteria for XAFS experiments and analyses as well as to discuss new data formats, databases and ideas for data deposition. The workshop also included discussion of recent improvements in technique and experimental procedures, the requirements of third-generation synchrotron radiation sources, and the opportunities afforded by future light sources. The workshop was co-organized by the IUCr XAFS Commission (Chair: Professor Isabella Ascone), the Synchrotron Radiation Commission (Chair: Professor Soichi Wakatsuki), the IXAS (International X-ray Absorption Society; Chair: Dr Hiroyuki Oyanagi), the IMSS (Institute of Materials Structure Science) and the JXS (Japan XAFS Society; Chair: Professor Kiyotaka Asakura). It was initially planned to hold the workshop in April 2011, but these plans were derailed by the disastrous earthquake that hit east Japan on 11 March 2011. The venue, the Photon Factory in Tsukuba, located very near to the epicenter, was heavily damaged, and the workshop was postponed until December 2011. Despite the disaster, and economically adverse situations such as the high level of the yen and an ongoing Euro crisis, 71 people including 25 from outside of Japan (USA, UK, France, Italy, Germany, Canada, Australia, Korea, China and Thailand) met for two days and enthusiastically discussed XAFS spectroscopy and its future.

The workshop was held with five oral sessions and one poster session.

S1: Experimental protocol and standardization of XAFS set-ups especially in bio-materials.

S2: Data formats and data library or data deposition method.

S3: New challenge to advanced techniques and beamlines.

S4: XAFS in green technology (science and technology related to environments and energy generations/savings): requirements for industrial use.

S5: Future prospects and demands on XAFS beamlines.

In order to maximize the productivity of the workshop, specific focus areas such as biological and green materials were selected. Parallels were drawn with the field of protein crystallography, which has well established protocols and procedures, with standards for automation, monitoring for radiation damage and data handling and analysis.

For XAFS analysis and experimental set-up, discussions concluded that experimentalists must be increasingly vigilant to maintain standards for measurements, such as dark-current corrections, dead-time corrections for solid-state detectors, and accurate energy calibration. Facility members were charged with the responsibility of listing beamline specifications and standardized procedures for accurate measurements, and routine regular checks of the operation of each XAFS beamline. Discussions noted that automation of data acquisition can maximize the productivity of high-throughput measurements, and is also potentially another way to ensure accurate measurements. The importance of tutorials and workshops held by the XAFS community was also emphasized, and several new techniques including time-resolved XAFS were discussed.

One major goal of the workshop was to lay the groundwork for standards of data deposition through discussion of data formats, data deposition and databases. This is increasingly needed since advanced experiments such as time-resolved or two-dimensional measurements can provide enormous quantities of data, with very large numbers of individual spectra. Several data formats including XDI, xasCIF and NEXUS were proposed and discussed. Further discussion is on-going, coordinated by a data archive working group which is comprised of core workshop participants. This working group is open, and anyone who is eager to join is welcome. Data deposition is still a complex problem, and to date the working group has not arrived at a consensus but will continue to reach it. Databases for standard compounds will be established, and the activities of the JXS were presented.

The following agreements were ratified at the workshop:

- (i) The IUCr XAFS Commission and the IXAS agreed to cooperate.
- (ii) Establishment of good standards and criteria are essential for the XAFS community.
- (iii) These standards should be discussed further at appropriate venues.
- (iv) Working groups focused on different areas of the workshop are in the process of being launched.

We will continue our efforts to establish standards and criteria through discussions held at the XAFS15 conference in Beijing 2012.

We would like to acknowledge all those who helped organize the Q2XAFS2011 meeting. We extend special thanks to the staff of the Photon Factory, who not only worked exceptionally hard in recovering from the earthquake, but also somehow found time to prepare and manage the workshop.



Conference photograph. (Courtesy of KEK.)

Invited speakers and their titles:

I. Ascone (ENSCP), Toward the standardization of BioXAS.

C. T. Chantler (University of Melbourne), A step toward standardization: development of accurate measurements of X-ray absorption.

R. Frahm (University of Wuppertal), Quick XAFS techniques: current status and new challenges at PETRA III.

G. George (University of Saskatchewan), BioXAS beamlines at the Canadian Light Source.

P. Glatzel (ESRF), Opportunities and traps of hard X-ray photon-in/photon-out spectroscopy.

J. Hester (ANSTO), Imaging a cif-based XAFS data exchange framework.

B. Hedman (Stanford University), Structural molecular biology/XAS beamline: experiences at SSRL.

K. Hodgson (Stanford University), Recent developments with the LCLS X-ray FEL at SLAC and prospects for future science.

P. Lay (University of Sydney), Metal speciation in biological systems with XANES and XAFS.

A. Marcelli (INFN), An advanced beamline for XAS and IR simultaneous time resolved experiments: a new approach to characterize non equilibrium phenomena.

S. Diaz-Moreno (Diamond), XAFS data collection: calibrations.

M. Newville (University of Chicago), XAFS data library for standard data on model compounds.

S. Pascarelli (ESRF), Energy-dispersive XAS: worldwide context.

B. Ravel (NSLS), A data interchange standard for XAS and related spectroscopies.

G. Sankar (The Royal Institution of Britain), Insight through *in situ* XAS studies of catalytic materials.

V. A. Sole (ESRF), HDF5 NeXus and beyond: approach to standard data format.

E. Welter (DESY), Ideas for assuring data quality and comparability at the new PETRA III EXAFS beamlines.

M. Nomura (Photon Factory), Toward the standardization of XAFS, transmission mode XAFS set-up.