Q2XAFS 2023 | International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy Closed Session Saturday 19th August 2023 | University of Melbourne School of Physics |GOSS Level 6. Conference Room Level 7 www.q2xafs.melbourne

The Journal for the Proceedings is Radiation Physics and Chemistry, as advertised earlier. Submission is already open. This will be a Special Issue of the journal. The senior Guest Editor is Peter Kappen. Submissions are required by April 2024.

Outcomes and Actions on the basis of the invited talks and the discussions on the Saturday meeting.

Chris Chantler, Sofia Diaz-Moreno, Kiyotaka Asakura¶
¶ with notes, edits, comments from Chris Chantler, Sofia Diaz-Moreno, Chanh Tran, Martin de Jonge, Giuliana Aquilanti, Valerie Briois

- Discussion topics 1 [Data Format] and 2. [Data and Metadata – Ontology, Semantics]

Action:
A Working Group would be formed to discuss and direct both of these priorities. The Working Group would be chaired by **Matt Newville** and should include representatives from different institutions such as synchrotrons and lab sources and expert users (Elettra, Soleil, ESRF, Gerry Seidler, ...). Specifically included because of their major work already on this, especially recently and in their talks, were: Ed Welter, Hitoshi Abe, Diego Gianolio, Abjiheet Gaur, Matt Newville, Shelly Kelly, Chanh Tran, Chris Chantler. Nobody would be excluded, but we should avoid double representation, as we need to be as diverse a working group as possible. Matt will include GitHub and multiple periodic zooms and emails according to time-zone challenges as he thinks appropriate.

Hence, in principle, this might produce: an Ontology and Dictionary, in agreement with the whole community, for a format-agnostic representation of the community [for XAFS, XANES, EXAFS]; and a mechanism representing all parties including at the Q2XAFS meeting and attendees, for the value and application of formats. The working group should work in close collaboration with the members of the CXAFS commission that are tasked to produce an on-line dictionary as requested by the EC of the IUCr (Anna Wolska and Eli Stavitski). Although there is not a hard deadline, it is expected that a progress report will be presented at the next Q2XAFS (see below).

- Discussion topic 3 [Summary, status of key extant spectral databases and repositories]

Action:
A paper would be prepared for submission to the Proceedings addressing this led by **Giannantonio Cibin** and **Abjiheet Gaur**, and will include Hitoshi Abe, Matt Newville, and Ichii-san. (Post-meeting note: it was suggested that **Hitoshi Abe** and **Abjiheet Gaur** would lead this, with Giannantonio, Ichii-san and Matt as co-authors.)

The paper should include a Table of all known Databases and their status; comments about quality criteria, and possible comments about structure, ongoing support, maintenance, interoperability and funding. An invitation to be involved might be extended to representatives of all databases.

- Discussion topic 4 [Round Robin]

Action:

Ed Welter has been leading this since the paper calling for the Round Robin. He is hopeful and expecting that at least 10 more labs / beamlines will contribute before December. This is an action item for those beamlines and any others interested. He will process all the spectra returned; the results will be published as a proceeding. During the meeting, a discussion arose regarding the terms and conditions of the round robin exercise. We previously agreed that the data are in Ed's hands for an evaluation of reproducibility in an anonymous way. People from the beamlines who participated in the Round Robin did it under these agreed conditions. The data are not to be shared with everyone else. Following the report of the results, this exercise will provide a confidence level that can be given in the measurement and analysis of the same sample (distance, coordination, S02…).

There was a brief discussion about the next Round Robin[s] including powder samples, either made in one lab, and distributed; or made in local labs; or using standard reference powders; and about the multiple standards of mounting which tend to be regionally based. Gerry Seidler will liaise with Ed Welter and the proponent group regarding sample preparation; Gerry suggested that his undergraduate students could prepare a series of pellets to be part of the RR second phase. As a possible additional follow-up, the assessment of how human approach or software affects the results of the analysis could be considered, as was raised in the original proposal.

- Discussion topics 5 and 6 [Most important approaches to quantify uncertainty in XAS/ XANES/ … and specific comments and recommendations on Dark Current, Blank Measurement, implementations …

Actions:

1. **Chanh Tran** would lead a summary publication for the Proceedings based upon his and Martin's talks and other contributions from the Q2XAFS speakers. He could include any other details as he might think fit.
2. A Working Group focussed on scanning type and mechanism – step scanning, continuous scanning and quick-exafs monochromators – was proposed. The working group will be led by **Giannantonio Cibin** and will include representatives from as many facilities as possible: Simon Bare (SSRL), Valerie Briois (Soleil), Giuliana Aquilanti (Elettra), Matt Newville (APS), Amelie Rochet (Sirius), Hitoshi Abe (Spring-8), Wantana Klysubun (Thai synchrotron), Ed Welter (Petra), … The working group will review aspects such as synchronization of signals, mechanics, acquisition strategies, etc. The timeline for recommendations and report were not yet defined.

- Discussion topic 7 [ML, AI, MCR-ALS]

Action:
Valerie Briois would lead a publication for the Proceedings, particularly on MCR-ALS following her talk, and particularly with Janis Timoshenko, but not excluding others as she feels appropriate.

- Discussion topic 8 [X-ray spectroscopy from Complementary theoretical methods]

Action:
Ritimukta Sarangi would lead a publication for the Proceedings, particularly on work reflected in her talk. *[Ritimukta Sarangi agreed to this in absentia.]*

It was acknowledged that this was a very important and large area of interest for the community, and that we currently do not have a well-defined framework to address this. It may be a subject of a future Q2XAFS meeting.

- Discussion topic 9 [Challenges and approaches for fragile / radiation-sensitive samples and [novel] approaches]

Actions:
1. **Ruwini Ekanayake** would be recommended to write up a paper with report and recommendations on this topic, reflected in her talk*. [Ruwini will be contacted after the meeting.]*
2. There will be a Working Group set up and led by **Ritimukta Sarangi**. Of those present, Sofia Diaz-Moreno and Giuliana Aquilanti showed an interest to be part of this working group. It should include representatives from each synchrotron, and members of the community that have contributed to this area. The working group will discuss and then report on beam-fragile systems, approaches to mitigate radiation damage, and possible ways to predict which samples will be mostly affected. *[Ritimukta Sarangi agreed to this in absentia.]*

- Discussion topic 10 [Challenges and approaches for Heterogeneous Catalysis]:

Action:
Simon Bare spoke on this, reflecting recent work by a large group in catalysis centred in the US, which is intended to lead to a publication. It was agreed that Simon Bare would be welcomed to present or summarise any of this in a publication for the Proceedings, in as much as there were no conflict with the other work. It was suggested that should it be appropriate; Shelly Kelly was also part of that group and could be a co-author or involved in the publication or report. Care should be taken to not set a global recommendation for work in this area unless (Post-meeting note: Valerie Briois talked to Simon as she would like to participate in the publication of those challenges and approaches in Catalysis. She has suggested to increase the author list, so a more international representation is drawn in)

- Discussion topic 11 [Extreme Conditions T, P, [t]]:

Action:
A paper would be prepared for submission to the Proceedings addressing this, led by **Giuliana Aquilanti**, who presented this. Giuliana Aquilanti will seek additional co-authors if appropriate.

- Discussion topic 12 [Photon-in, photon-out spectroscopies]:

Actions:

1. A paper would be prepared for submission to the Proceedings addressing this led by **Simo Huotari, Gerald Seidler** and **Sofia Diaz-Moreno**, possibly on 'Guidelines for Reporting Photon-in, photon-out spectroscopies', and possibly as a User Guide. The authors will decide if including tender photon-in/photon out.
2. **Simo Huotari** to decide if he will prepare a proceeding on XRS.

- Discussion topic 13 [Dilute Systems, Noise]:

Actions:

1. A paper would be prepared for submission to the Proceedings addressing this led by **Wantana Klysubun**, based around her presentation. Free to include any co-authors as always.
2. A Working Group would look towards all issues relating to Tender X-ray Spectroscopy, possibly with a view to presenting an initial Overview paper or report to look towards a Review later. This would be led by **Diego Gianolio**, with Wantana Klysubun, Simon Bare, Giuliana Aquilanti, Hitoshi Abe, somebody from Lucia beamline (Soleil), from Solaris, Chris Glover (ANSTO) and any others interested.

There was a request / suggestion that Tender XAFS might be a topic of the next Q2XAFS. And another that there might be a topic of the next Q2XAFS on Fluorescence data collection.

- Discussion topic 14 [Laboratory-based XAFS]:

Action:
A paper would be prepared for submission to the Proceedings addressing this led by **Gerald Seidler**, based around his presentation, with Simo Huotari.

- Discussion topic 15 [Opportunities with the International Tables for Crystallography, Volume I: XAS]:

Action:
A paper would be prepared for submission to the Proceedings addressing this led by **Chris Chantler**, based around his presentation, addressing a suite of Q2XAFS topics discussed in the Q2XAFS meeting. Chris would invite Federico Boscherini and Bruce Bunker as the other Editor in Chief of the encyclopaedia.

Other Actions: ***Kiyotaka Asakura*** *proposed that there be a Q2XAFS meeting in Japan, possibly 2024 or maybe 2025. This was received very positively, and much discussion surrounded the most appropriate month for it to be scheduled in, so that the next action*

on this will be a poll which Kiyotaka-san will distribute to all speakers and attendees of Q2XAFS, and to IXAS and CXAFS. The poll will be done in time slots of 15 days, starting on the 15th of August 2024 up to the 15th of December 2024.

Chanh Tran suggested that the next Q2XAFS meeting should be opened by an overview presentation summarising the action plans and achievements of this meeting.

Session outline

Session 1: Sharing and re-using XAS data

- Data formats (plain text, XDI, xasCIF, NeXus/HDF5, CIF)
- Metadata (Essential meta data, ontology of XAFS related terminology)
- XAFS databases
- Comparability of XAFS data (Round Robin)

Session 2: Improving the interpretation of XAS data

- Quantification of uncertainties during EXAFS data evaluation and propagation of uncertainties
- Quantification and correction of experimental uncertainties (dark currents, dead time etc.)
- Quantifying uncertainties in XANES evaluation methods (PCA etc.)
- Novel methods (Machine Learning, AI…)

Session 3: Improving the quality of XAS measurements

- Bio and other fragile samples (beam damage)
- Extreme conditions (ultrafast, high-pressure, in-operando)
- Fast measurements (Q-XAFS, dispersive XAFS)

Session 4: Improving the reporting of XAS results

- General reporting guidelines for XAS publications
- IUCr and CXAFS reports
- Assessing experimental data quality
- Including uncertainties in pre-processed data and reported results
- Specific challenges and reporting for photon in/photon out spectroscopies
- Specific challenges and reporting for lab-based XAFS

Note: Q2XAFS speakers are listed, and may be indicative of key people for Discussion, Working Groups, Co-authors for Reports or Papers; but do not exclude eager volunteers attending Q2XAFS and the Closed Session or other suggestions; except insofar as to define a finite timeline for objectives.

Program
Saturday, 19th August 2023
Geoff Opat Seminar Room, Level 6.

Breakout Room Conference Room Level 7.

10:00 am	Opening	Chris Chantler	Sofia Diaz-Moreno	Matt Newville	
10:15 am	Welcome and Overview of Q2XAFS meeting	Kiyotaka Asakura			
10:40 am	Discussion 1: Data Formats [1.1]	Q2XAFS Speakers: James Hester Hitoshi Abe Abhijeet Gaur Chanh Tran Matthew Newville Shelly Kelly	Moderator: Chris Chantler Additional Volunteers / Contributors: ?	Outcome: Paper on current, parallel developments, prospects, convergence.	
	a) For retention of data				
	b) For reporting, papers			a≠b=c=d?	
	c) For robust cross-platform analysis			Development of readers for any [all] formats	
	d) For Databases				
	Discussion 2: [Data and] Metadata [1.2]	Q2XAFS Speakers: Ed Welter Hitoshi Abe Gerald Seidler Abhijeet Gaur Shelly Kelly Chanh Tran Chris Chantler		Outcome: Paper on data and metadata and convergence for any format, especially for b,c,d.	
	a) b) c) d)				
	Discussion 3: Summary, status of key extant spectral databases and repositories [1.3]	Q2XAFS Speakers: James Hester Hitoshi Abe Abhijeet Gaur Giannantonio Cibin Sofia Diaz-Moreno [or delegate]		Outcome: Working Group and Paper. Funding, Structure and Support.	
	a) 'Local synchrotron depository'				
	b) 'Uncritical'				
	c) 'Robust, reference and portable'				
	Discussion 4: Round Robin Action Plan and Priority, Timeline [1.4]	Q2XAFS Speakers: Ed Welter Hitoshi Abe Gerald Seidler		Outcome: Action Plan, Timeline, Team. Manpower. Maybe status report.	
	Discussion 5: Most important approaches to quantify uncertainty in XAS	Q2XAFS Speakers: Martin de Jonge Chanh Tran		Outcome: Recommendations	

	/ XANES / pre-edge / XAFS / Transmission, Fluorescence [2.1]	Chris Chantler		Paper and feed into 1,2,3,4.	
	Discussion 6: Specific comments and recommendations on Dark Current, Blank measurement, ~~scan type,~~ mechanisms for implementation [2.2]	Q2XAFS Speakers: Diego Gianolio Martin de Jonge Chanh Tran Chris Chantler		Outcome: Recommendations Paper and feed into 1,2,3,4.	
1 pm -2 pm	Lunch on Lygon Street				
2 pm	Discussion 7: Novel Augmented neural network methods: ML, AI, report [2.3]	Q2XAFS Speakers: Valerie Briois Janis Timoshenko		Outcome: Applications and prospects paper[s]	
	Discussion 8: X-ray Spectroscopy from complementary theoretical methods [2.4]	Q2XAFS Speakers: Ritimukta Sarangi		Outcome: Applications and prospects paper[s], path to the future?	
	Discussion 9: Challenges and approaches for fragile / radiation-sensitive / bio samples and novel approaches [3.1]	Q2XAFS Speakers: Ruwini Ekanayake Ritmukta Sarangi Simon Bare		Outcome: Applications and prospects paper	
	Discussion 10: Challenges and approaches for Heterogenous Catalysis [3.1?]	Q2XAFS Speakers: Simon Bare		Outcome: Applications and prospects paper	
	Discussion 11: Challenges and approaches for Extreme Conditions [High T,P] [3.2]	Q2XAFS Speakers: Giuliana Aquilanti		Outcome: Applications and prospects paper	
	Discussion 12: Challenges and approaches for Photon-in, Photon-out spectroscopies [4.5]	Q2XAFS Speakers: Sofia Diaz-Moreno Simo Huotari	Chris Chantler	Outcome: Applications and prospects paper	
	Discussion 13: Challenges and approaches for Dilute Samples? [3.2?]	Q2XAFS Speakers: Wantana Klysubun	Chris Chantler	Outcome: Applications and prospects paper	
	Discussion 14: Challenges and approaches for Lab-based XAS [4.6]	Q2XAFS Speakers: Gerald Seidler, Simon Bare			
	Discussion 15: Opportunities with the International Tables for Crystallography Volume I: XAS [4.2]	Q2XAFS Speakers: Chris Chantler		Outcome: Report Paper and feed into 1,2,3,4...	
4:30 pm	Close				

Other key players in last decade not otherwise listed above:
1.1 Bruce Ravel, USA, Athena, XDI. Individual Beamline and Synchrotron Formats. All software analysis package authors.
1.2 Matt Newville, Bruce Ravel, Ritimukta Sarangi [Bio], Kiyotaka Asakura
1.3 Kiyotaka Asakura, Masao Kimura
1.4 Chris Chantler, Bruce Bunker, Matt Newville, Kiyotaka Asakura, earlier: Shelly Kelly, Simon Bare
2.1 Sakura Pascarelli, Paola d'Angelo, Ritimukta Sarangi, Grant Bunker, Matt Newville, Frank Bridges, Steve Heald
2.2 Giannantonio Cibin, fluorescence dead time corrections, Sofia Diaz-Moreno (Bragg peaks)
2.3 Increasingly popular [!]
2.4 Advanced experimental and theoretical groups. Chantler, Rehr, Kas, Cicco, Bianconi, …
3.1
3.2 Federico Boscherini, Sakura Pascarelli, Joel Brugger
4.1 See 1.2, 1.3 ,1.4
4.2 Bruce Bunker, Federico Boscherini, ITC Volume I authors.
4.3 See 1.2, 1.3, 2.1, 2.2
4.4 See 1.2, 1.3, 2.1, 2.2
4.5 Pieter Glatzel, XR-HERFD Chris Chantler
4.6 Serena De Beer, Tonya Vitova, Jan-Dierk Grunwaldt

Note directly relevant selected documents:
Report of the International XAFS Society Standards and Criteria Committee, D E Sayers, Chair, 2000
Error Reporting Recommendations: A Report of the Standards and Criteria Committee, 2000

Selected Publications and authors from Q2XAFS I
Ascone, Asakura, George, Wakatsuki, J Synch Rad 19 (2012) 849
Chantler, Barnea, Tran, Rae, J Synch Rad 19 (2012) 851
Diaz-Moreno, J Synch Rad 19 (2012) 863
Ravel, Hester, Sole, Newville, J Synch Rad 19 (2012) 869
George, Pickering, Pushie, Nienabar, Hackett, Ascone, Hedman, Hodgson, Aitken, Levina, Glover, Lay, J Synch Rad 19 (2012) 875-886

Biancini, Glatzel, J Synch Rad 19 (2012) 911
[Stotzel, Lutzenkirchen-Hecht, Grunwaldt, Frahm, J Synch Rad 19 (2012) 920-929]

Hester Data Science Journal 15 (2016) 1-17

Selected Publications and authors from Q2XAFS III
Diaz-Moreno, Strange, J Synch Rad 25 (2018) 918-919
Schalken, Chantler, J Synch Rad 25 (2018) 920-934
Chantler, Bunker, Abe, Kimura, Newville, Welter, J Synch Rad 25 (2018) 935-943
Sarangi, J Synch Rad 25 (2018) 944
Figueroa, Beniz, Mauricio, Piton, Parry, Cibin, J Synch Rad 25 (2018) 953
Mangold, J Synch Rad 25 (2018) 960
Asakura, Abe, Kimura, J Synch Rad 25 (2018) 967
Abe, Aquilanti, Boada, Bunker, Glatzel, Nachtegaal, Pascarelli, J Synch Rad 25 (2018) 972

Shelly's round robin: Kelly, Bare, Greenlay, Azevedo, Balasubramanian, Barton, Chattopadhyay, Fakra, Johannessen, Newville, Pena, Pokrovski, Proux, Priolkar, Ravel, Webb, 2010 online