Q2XAFS 2023 | International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy

17th – 18th August 2023 | Australian Synchrotron – ANSTO | www.q2xafs.melbourne

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

Q2XAFS 2023 | International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy

17th – 18th August 2023 | Australian Synchrotron – ANSTO | www.q2xafs.melbourne

Program

Note: each presentation is 20+5 minutes in length

Day 1 | Thursday, 17th August 2023

08.30 h	**Registration**	
09.00 h	**Welcome** Acknowledgement of Country	Jessica Hamilton
	Q2XAFS 2023 - Opening	Danielle Martin, *Senior Principal Scientist – Australian Synchrotron*

09.10 h	**Session 1 | Sharing and re-using of XAFS data**	***Chair: Chris Chantler***
	1.1 First experiences and results from an inter-laboratory round robin test of XAFS spectroscopy measurements.	Edmund Welter, DESY
	1.2 XAS Reference Database under DAPHNE4NFDI.	Abhijeet Gaur, KIT
	1.3 Sharing XAFS data and repositories: where to go?	Giannantonio Cibin, Diamond LS
10.25 h	*Morning tea*	
10.55 h	1.4 Formats for Sharing XAFS Data, Metadata, and Analysis Results.	Matthew Newville, University of Chicago
	1.5 Quantity yields quality, using and building XAFS database.	Hitoshi Abe, KEK
	1.6 Making a comprehensive XAFS data standard actually happen.	James Hester, ANSTO
12.10 h	Session 1 – discussion and conclusion	
12.30 h	*Lunch*	

Principal Sponsors (Q2XAFS is co-organised by members of, and sponsored by, ANSTO (host) and IUCr)

ANSTO IUCr

Silver Sponsors

LA TROBE UNIVERSITY | LA TROBE INSTITUTE FOR MOLECULAR SCIENCE | MIRION TECHNOLOGIES

13.15 h	**Session 2 | Improving the interpretation of XAS data**	***Chair: Sofia Diaz-Moreno***
	2.1 Notes from another world: Precise and accurate X-ray attenuation measurements in the vicinity of the absorption edge.	Martin de Jonge, ANSTO
	2.2 A 20-year journey hunting down uncertainties and extracting physical information in Absorption and Fluorescence X-ray Spectroscopy.	Chanh Tran, La Trobe University
	2.3 Improving the interpretation of XAS data using artificial neural networks.	Janis Timoshenko, FHI Berlin
	2.4 Multivariate Curve Resolution - Alternating Least Squares (MCR-ALS) Analysis applied to XAS data: Principles, Strength, Weakness and Strategies to overcome intrinsic limitations.	Valérie Briois, SOLEIL
14.55 h	Session 2 – discussion and conclusion	

15.15 h	**Tour to the Australian Synchrotron (focus on XAS beamlines)**
16.00 – 18.00 h	**Afternoon tea & Poster session**

Q2XAFS 2023 | International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy

17th – 18th August 2023 | Australian Synchrotron – ANSTO | www.q2xafs.melbourne

Day 2 | Friday 18th August 2023

09.00 h	**Welcome – Day 2**	Valerie Mitchell

09.05 h	**Session 3 | Improving the quality of XAS measurements**	***Chair: Matthew Newville***
	3.1 A new protocol for monitoring radiation damage of XAS data, multiple datasets and fitting of XAS measurements with propagated uncertainties.	Ruwini Ekanayake, KIT
	3.2 Comparing the quality of XAFS data collected with different acquisition rates.	Diego Gianolio, Diamond LS
	3.3 XAFS at extremes: last trends.	Giuliana Aquilanti, Elettra
	3.4 Winds of change at the XAS beamline in Melbourne	Bernt Johannessen, ANSTO
10.45 h	*Morning tea*	
11:15 h	3.5 Data quality and standards in x-ray Raman scattering spectroscopy	Simo Huotari, University of Helsinki
11.40 h	Session 3 – Discussion and conclusions	

(Day 2 program continues next page)

Q2XAFS 2023 | International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy

17th – 18th August 2023 | Australian Synchrotron – ANSTO | www.q2xafs.melbourne

12.00 h	**Session 4 | Improving the reporting of XAFS results**	***Chair: Chanh Tran***
	4.1 Trends in X-ray absorption data sharing, reproducibility, and measurement and interpretation challenges.	Shelly Kelly, APS
	4.2 From data collection to reporting in photon-in/photon-out spectroscopies.	Sofia Diaz-Moreno, Diamond LS
12.50 h	*Lunch*	
13.40 h	4.3 Learning more from X-ray Spectroscopy with Theoretical Methods.	Ritimukta Sarangi, SLAC
	4.4 Best Practice for High Data Quality in Laboratory-Based X-ray Absorption Spectroscopy.	Gerald Seidler, University of Washington
	4.5 Addressing Rigor and Reproducibility in Heterogeneous Catalysis: XAS.	Simon Bare, SLAC
14.55 h	*Afternoon tea*	
15.25 h	4.6 Assessing data quality and experimental challenges at medium-energy K-edge absorption (1.5-4 keV) for dilute samples.	Wantana Klysubun, SLRI
	4.7 IUCr, ITC I, IXAS, XERT, Hybrid, Measurement Standards, Reporting Guidelines and Soliloquy on Q2XAFS 2023.	Chris Chantler, University of Melbourne
16.15 h	Session 4 – Discussion	

16.35 h	**Poster Awards presentation**	
	Q2XAFS 2023 Close	Sofia Diaz-Moreno, *Co-Chair – Q2XAFS23 International Organising Committee*

17.00h	**Departure to Melbourne CBD**
evening	**Workshop dinner**

FINAL; 09/August 23

Principal Sponsors (Q2XAFS is co-organised by members of, and sponsored by, ANSTO (host) and IUCr)

Silver Sponsors