The annual event dedicated to
the ESRF user community and to
user science

ESRF
USER MEETING
5-7 February 2024

5 FEBRUARY
11 Tutorials for Users

6 FEBRUARY
Plenary Session
Commercial Exhibition
Poster Session

7 FEBRUARY
4 User-Dedicated
Microsymposia

CONTENTS

ESRF USER ORGANISATION

ESRF
The European Synchrotron

EPN Science Campus

71 avenue des Martyrs,
38000 Grenoble

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esrf_synchrotron

User Meeting 2024

Monday 5 February – Tutorials

T1. Volume image analysis of tomographic data
T2. Structural Biology BAG meeting
T3A. Meet the Structural Biology scientists on the beamlines
T3B. Demystifying the Structure-tO-Solution (SOS) pipeline: A comprehensive tutorial on its current components
T4. How to write a news article on a scientific publication
T5. Data reduction for scattering experiments using pyFAI
T6. XAS data analysis – Common session
T7A. Introduction to the XAS technique and to the LISA beamline
T7B. Ab initio simulation of X-ray absorption spectroscopies using FDMNES
T8. XPCS: X-ray Photo Correlation Spectroscopy
T9. Nuclear resonance applications at the nanoscale including hands-on practical

Tuesday 6 February – Plenary Session

Venue: ESRF Auditorium

Administrative Assistants: Sabine Schreiber – Sabine Persico – Sonya Girodon
Tel: +33 (0)4 76 88 25 52 / 23 58 / 28 80 – usermeet@esrf.fr

Wednesday 7 February – Microsymposia

UDM1 Towards filming macromolecular movies at the ESRF-EBS
Venue: **IBS Seminar Room**

Administrative Assistant: Claudine Romero
contact: udm1-um24@esrf.fr   Tel: +33 (0)4 76 88 20 27

UDM2 Machine learning and databases in X-ray spectroscopy
Venue: **ESRF Auditorium**

Administrative Assistant: Eva Jahn-Feppon
contact: udm2-um24@esrf.fr   Tel: +33 (0)4 76 88 26 19

UDM3 The complementary use of diffuse and inelastic X-ray scattering
Venue: **ESRF MD-1-21**

Administrative Assistant: Eleanor Ryan
contact: udm3-um24@esrf.fr   Tel: +33 (0)4 76 88 19 92

UDM4 Introduction to the ESRF HOAHub: creating an Atlas of Human Organs in Health, Ageing and Disease
Venue: **CIBB Meeting room**

Admin. Assistant: Luce Chabert/ Marion Glueckert
contact: udm4-um24@esrf.fr   Tel: +33 (0)4 76 88 20 13

ESRF USER MEETING 2024
OVERALL PROGRAMME

MONDAY 5
11 TUTORIALS

8:15 9:00	📋	Registration *Central Building* *WELCOME COFFEE*

9:00		
	TUTORIALS	
12:00		

LUNCH BREAK

| 13:00 14:00 | 📋 | Registration *Central Building* |

14:00		
	TUTORIALS	
18:00		

| 18:00 20:30 | ☕ | *BUFFET DINNER* *In Marquee* |

TUESDAY 6
PLENARY SESSION

8:15 9:00	📋	Registration *Central Building* *WELCOME COFFEE*

9:00	Opening & Welcome
9:05	🔍 Giovanna Fragneto
9:50	🔍 Beatrice Vallone

COFFEE BREAK

11:00	🔍 Francesco Sette
11:45	ESRF-EBS Facility Report

LUNCH BREAK

14:00	🔍 Andrei Petukhov
14:45	🔍 Andreas Schaefer

COFFEE BREAK

16:00	Poster Clips
17:00	Young Scientist Award
17:50	Conclusion

| 18:00 22:00 | ☕ | *POSTER SESSION & COCKTAIL DINNER* *In Marquee / Common Building Restaurant* |

WEDNESDAY 7
4 USER-DEDICATED MICROSYMPOSIA

8:15 9:00	📋	Registration *At Event Venue* *WELCOME COFFEE*

UDM1
IBS Seminar Room

8:50 18:00	Towards filming macromolecular movies at the ESRF-EBS

UDM2
ESRF Auditorium

9:00 17:30	Machine learning and databases in X-ray spectroscopy

UDM3
ESRF MD-1-21

8:55 16:00	The complementary use of diffuse and inelastic x-ray scattering

UDM4
CIBB Meeting room

9:00 13:00	Introduction to the ESRF HOAHub: creating an Atlas of Human Organs in Health, Ageing and Disease

END OF MEETING

Practical information

Badge information

You have been given a **BADGE** at the site entrance: <u>**this badge is strictly personal**</u> and due to the strengthened security measures, **you MUST wear your badge at all times on site over the whole period of the event**. It is your pass for the site entrance and, on site, for the Guesthouse and the canteen. <u>**Please note that access to the Experimental Hall is strictly forbidden**</u>.

Lunches

Lunches **are served** from

11:30 - 13:30

ground floor - restaurant

11:30 - 13:00

1st floor - restaurant

Please present your **USER MEETING BADGE** to the cashier.

Monday 5 February

Buffet Dinner

18:00 – 20:30

under the marquee

Tuesday 6 February
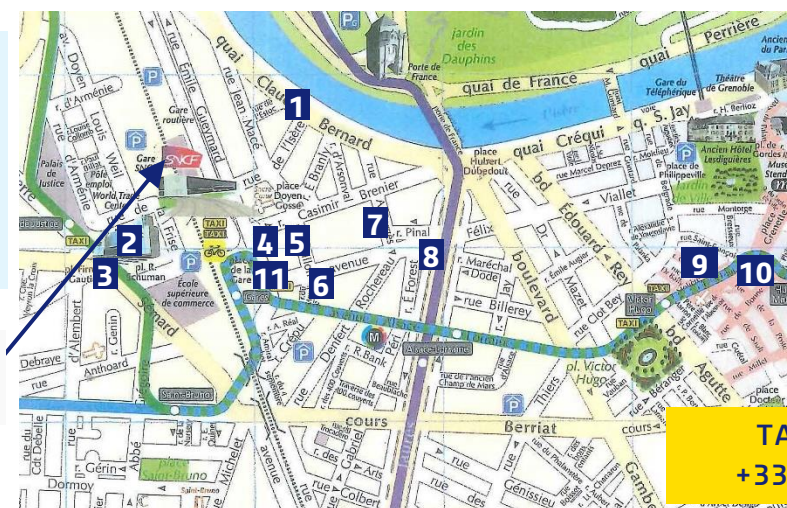
Poster Session & Cocktail Dinner

18:00 – 22:00

under the marquee / Common Building Restaurant

Hotels in the center of Grenoble

HOTELS

1 Ibis Grenoble Gare
2 Novotel Grenoble Centre
3 Hotel Europole
4 Residhotel Central'Gare
5 Maison Barbillon

Train Station
(SNCF)

HOTELS

6 Greet Hotel (ex Hotel des Alpes)
7 Hotel Gloria
8 Hotel Ibis Styles Gare
9 Ibis Grenoble Centre Bastille
10 Hotel de l'Europe
11 Brit Hotel Suisse et Bordeaux

TAXI GRENOBLOIS
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TWEETING DURING THE MEETING?

Don't forget to add the hashtag **#ESRFUM2024** to your messages. And follow the ESRF on social media:
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For further information, please contact: Sabine Schreiber, Sabine Persico, Sonya Girodon
ESRF Central Building – Room 004 (ground floor) – Tel: +33 (0)476 88 25 52 / 23 58 / 28 80

List of Exhibitors
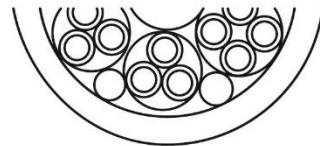
Exhibitors attending the
2024 ESRF User Meeting

ALCA TECHNOLOGY

www.alcatechnology.com

allectra

www.allectra.com

SPECIAL CABLES
CABLERIE SAB

www.sab-cable.com

DECTRIS
detecting the future

www.dectris.com

Exhibitors attending the
2024 ESRF User Meeting

www.edwardsvacuum.com

www.xhuber.com

www.pi.ws

www.pink.de/en/

https://symetrie.fr/

Exhibitors attending the 2024 ESRF User Meeting

https://torrscientific.co.uk/

www.vacuumfab.com

https://x-spectrum.de/

www.tsa.fr

www.zeiss.com

Tutorials

5 February 2024

- Overall Programme

User Meeting 2024 - Tutorials
Monday 5 February 2024

	TUTORIAL TITLE	ORGANISERS	TIME	VENUE
T1	Volume image analysis of tomographic data	Alexander Rack (ESRF)	09:00 - 17:00	MD-1-21
T2	Structural Biology BAG Meeting	David Flot (ESRF) Montserrat Soler Lopez (ESRF) Max Nanao (ESRF) Romain Talon (ESRF)	09:00 - 12:30	CIBB Seminar room
T3A	Meet the Structural Biology scientists on the beamlines		14:00 - 15:00	Guided tour: ID29-EBSL8, icOS, HPMX, BM29
T3A			15:00 - 18:00	Visitor Center discussion with beamline scientists
T3B	Demystifying the Structure-tO-Solution (SOS) pipeline: A comprehensive tutorial on its current components	Eaazhisai Kandiah (ESRF) Gregory Effantin (IBS)	14 :00 - 17 :00	CIBB Seminar room and visit to Cryo-EM facility
T4	How to write a news article about a scientific publication	Montserrat Capellas Espuny (ESRF)	12:15 - 13:45	Visitor Center (with Buffet)
T5	Data reduction for scattering experiments using pyFAI	Edgar Gutierrez Fernandez (ESRF)	14:00 - 17:00	Central Building 3rd floor room 337
T6	XAS data analysis – Common session	Kirill Lomachenko (ESRF)	09:00 - 12:00	Central Building Auditorium
T7A	Introduction to the XAS technique and to the LISA beamline	Francesco d'Acapito (CNR/ESRF) Alessandro Puri (CNR-IOM) Jacopo Orsili (Univ, Milano)	14:00 - 17:00	Experimental Hall Sect.07.5.02 room 07.5
T7B	Ab initio simulation of X-ray absorption spectroscopies using FDMNES	Yves Joly (CNRS)	14:00 - 17:00	Lob: BEL-1-01
T8	XPCS: X-ray Photo Correlation Spectroscopy XPCS: X-ray Photo Correlation Spectroscopy	Federico Zontone (ESRF) Yuriy Chushkin (ESRF) Marco Cammarata (ESRF)	14:00 - 16:30	EMBL Seminar room
T9	Nuclear resonance applications at the nanoscale including hands-on practical	Dimitrios Bessas (ESRF) Ilya Kupenko (ESRF) Aleksandr Chumakov (ESRF) Rudolf Rüffer	09:00 - 18:00	Experimental Hall Sect.18: room 18.1.11 and ID14

Plenary Session

6 February 2024

- Programme
- Abstracts of lectures

Plenary Session
Tuesday 6 February 2024

	MORNING SESSION	
09:00 – 09:05	Opening and welcome by the User Organisation – **Guillaume Morard**	
09:05 – 09:50	**Invited Speaker** *"Complementarity of neutrons and synchrotron radiation for the study of cell membranes"* **Giovanna Fragneto**, European Spallation Source ERIC, Lund, Sweden	Chair: **Beatrice Ruta** (UOC)
09:50 – 10:35	**Keynote Lecture 1** *"Determinants for iron uptake on ferritin and on the transferrin receptor"* **Beatrice Vallone,** Università di Roma « La Sapienza », Rome, Italy	Chair: **Alberto Martinelli** (UOC)
10:35 – 11:00	*Break*	
11:00 – 11:45	**Keynote Lecture 2** *"ESRF – Upgrade and EBS"* **Francesco Sette,** European Synchrotron Radiation Facility, France	Chair: **Tilman Grünewald** (UOC)
11:45 – 12:30	**ESRF-EBS Facility and Directors' Report** • Directors Of Research's report - **Michael Krisch and Gema Martinez Criado** • Latest news from ID14 - **Alexander Chumakov** • Latest news from the Sample environment support service - **Yves Watier**	
12:30 – 14:00	*LUNCH break*	

	AFTERNOON SESSION	
14:00 – 14:45	**Keynote Lecture 3** *"Bright insights into the nanoworld"* **Andrei Petukhov**, Debye Institute for Nanomaterials Science, Utrecht University, Netherlands	Chair: **Stefan Kowarik** (UOC)
14:45 – 15:30	**Keynote Lecture 4** *"X-ray tomography for Circuit Neuroscience – Towards X-ray Connectomics"* **Andreas Schaefer**, The Francis Crick Institute, London, United Kingdom	Chair: **Adriana Miele** (UOC)
15:30 – 16:00	*Break*	
16:00 – 17:00	**Poster Clips**	Chair: **Barbara Fayard** (UOC) **Matthias Bauer** (UOC)
17:00 – 17:50	**Young Scientist Award 2024** President: Jean Daillant, Soleil Synchrotron, Paris, France	Chair: **Guillaume Morard** (UOC)
17:50 – 18:00	Conclusion	
18:00 – 22:00	Poster Session, Poster Prize & Cocktail Dinner	

Complementarity of neutrons and synchrotron radiation for the study of cell membranes

G.Fragneto

Affiliation: European Spallation Source ERIC, Partikelgatan 2, SE-22484 Lund, **giovanna.fragneto@ess.eu**

The understanding of the function of cellular membranes requires the study of their structure and dynamics. Cellular membranes are complex assemblies of lipids and proteins. In particular, the lipid scaffold is composed by a large variety of lipid species and levels of chain unsaturation, often difficult to synthesise chemically. Because of this complexity, model membrane systems from simple lipid bilayers are often used for fundamental studies and those can profit from probes able to access different scales of size and time like thermal neutrons and synchrotron radiation. Since the pioneering neutron scattering work in the seventies on cell membrane structure, developments driven by constantly improving neutron instrumentation, coupled with development of measurement and analysis methods, have involved both the optimisation of samples towards more biologically relevant model systems including the use of more and more complex lipid mixtures up to natural extracts.

Here, we will focus on developments made in the last decades at the Institut Laue-Langevin in Grenoble, F, on developing model membrane systems and their use in interaction with different proteins, as well as the complementary studies with synchrotron radiation.

These will comprise the development of advanced models of biological membranes [1,2] including systems with hydrogenous and deuterated natural glycerophospholipid mixtures and their study with neutron and synchrotron radiation scattering techniques.
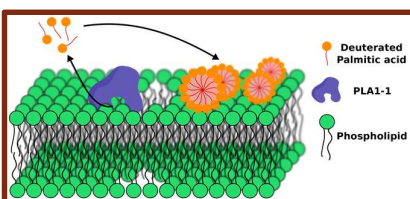

Figure 1: Cartoon of interaction of a phospholipase with lipid bilayers [3].

References

[1] G. Corucci, J. Coll. Int. Sci. (2023)

[2] Muckina et al. J. Coll. Int. Sci. (2021)

[3] G. Corucci PhD Thesis, UGA and ILL (2023)

Determinants for iron uptake on ferritin and on the transferrin receptor.

L.C. Montemiglio[1,2], C. Testi[1,3], P. Ceci[2], E. Falvo[2], M. Pitea[1], C. Savino[2], A. Arcovito[4], G. Peruzzi[3], P. Baiocco[3], F. Mancia[5], A. Boffi[1,3], A. des Georges[6], B. Vallone[1,2,].

[1]Dept of Biochemical Sciences Sapienza University of Rome, Italy, [2]CNR-IBPM, Rome, Italy [3]CNLS@Sapienza, IIT, Rome, Italy, [4]Università Cattolica del Sacro Cuore, Rome, Italy, [5]Columbia University Medical Center, New York, USA, [6]ASRC-CUNY, New York, USA
beatrice.vallone@uniroma1.it

Human transferrin receptor-1 (CD71) guarantees iron supply by endocytosis upon binding of iron-loaded transferrin and ferritin to CD71. Viruses and the malaria parasite exploit CD71 for cell invasion and epitopes on CD71 for interaction with transferrin and pathogenic hosts were recently identified. We provide the molecular basis of the human ferritin-CD71 interaction by the 3.9 Å resolution single-particle cryo-electron microscopy structure of their complex and by validating our structural findings in cellular context [1]. The structure of the H-Ft/CD71 complex revealed the specific sites on CD71 to be hooked by ferritin for physiological access to cell through the CD71 "iron door". Moreover, it accounts for a Tf-independent binding of ferritin to the receptor, allowing differential regulation of iron uptake, and indicates a physiological role for the CD71 apical domain, unassigned to date. The contacts between the heavy-chain ferritin and CD71 largely overlap with arenaviruses and Plasmodium vivax binding regions in the apical part of the receptor ectodomain [2,3]. Our data account for transferrin-independent binding of ferritin to CD71 and suggest that select pathogens may have adapted to enter cells by mimicking the ferritin access gate and it provides a sound structural basis to elaborate on the possibility of developing alternative ferritin-like anti-viral or anti-parasite therapeutic ligand, be it an antibody or a peptidomimetic capable of blocking the "common contacts" epitope on CD71 residue, and to further engineering ferritins as nanocarriers and theranostic agents.

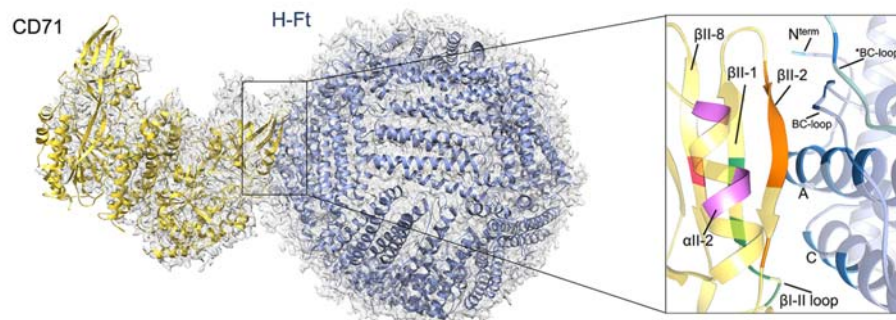Figure 1: The complex between human ferritin and the CD71 receptor and details of contact interactions.

References
[1] L.C. Montemiglio *et al. (*2019) *Nat Comm, 10(1)-1121.*
[2] A. Demogines, *et al.* (2013) *PLoS Biol*, 11(5), e1001571.
[3] J. Gruszczyk, *et al.* (2018) *Science*, 359(6371), 48-55.

ESRF – Upgrade and EBS

Francesco Sette

ESRF, 71 Avenue des Martyrs, 38000 Grenoble – France, **sette@esrf.fr**

The ESRF has been involved in a major reconstruction programme, which started in 2009 – about 20 years after the launching of the ESRF programme in 1988 – and comes to its formal end in 2023. This programme, referred to as the ESRF Upgrade Programme, is grounded on ESRF role and mission of pioneering synchrotron science to the benefit of society. After the successful launching and operation of the first third-generation synchrotron source and beamlines in 1992, which became model and reference of the present rich scenario of synchrotron sources around the world, the ESRF pointed out already since its *2004 User Meeting* the growing importance of convergence among X-ray imaging and microscopy methods with established X-ray science scattering and absorption techniques. These new opportunities had the potential to open completely innovative avenues on the exploration of the micro- and nano-world, enabling much more powerful investigations on the different structural hierarchies present in many complex materials and in living matter. To this purpose, new adapted concepts – enhancing X-ray source and instrument performance to explore with new enhanced spatial resolution condensed and living matter – had to be developed. These considerations rapidly developed into the Science Case supporting what then became the ESRF Upgrade Programme.

The implementation of the ESRF Upgrade Programme, divided in two phases – Phase I (2009-2015) and EBS (2015-2023), has enabled and determined an almost complete reconstruction of the ESRF facility, with 27 new beamlines, a new storage ring-based X-ray synchrotron source (EBS the Extremely Brilliant Source), and new scientific infrastructure and instrumentation. During these last few years, the new EBS storage ring came to operation with revolutionary performance, thus enabling and opening many new applications in X-ray science, and becoming the new role model for modern X-ray synchrotron sources around the world.

I will present a summary of the ESRF programme with some particular attention to the recent construction and commissioning of the EBS storage ring [1] and its impact in providing new opportunities to X-ray science and applications.

References
[1] – Raimondi, P., Benabderrahmane, C., Berkvens, P. *et al.* The Extremely Brilliant Source storage ring of the European Synchrotron Radiation Facility. *Commun Phys* **6**, 82 (2023). https://doi.org/10.1038/s42005-023-01195-z

Bright insights into the nanoworld

A.V. Petukhov

Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands **a.v.petukhov@uu.nl**

Structures of the scales from a nanometre to several microns are playing an increasingly important role in modern research. They are at the heart of nanomaterials and soft matter. Synchrotron radiation is able to provide crucial insights into the nanoscale structures, which can be gained in-situ and time-resolved.

One of the unmissable pillars of nanomaterials is quantum dots, i.e. semiconductor nanoparticles that are so tiny that their size strongly affects their properties. The discovery of synthesis routes to produce monodisperse quantum dots in the 80s and 90s was recently crowned by the 2023 Nobel Prize in chemistry. These pioneering works led to the development of a broad and active research field. By now, a broad spectrum of nanoparticles of different composition, size and shape can be produced and studied. I will illustrate some insights into the nanoparticle synthesis, which can be provided by synchrotron radiation.

The central concept in nanomaterials and soft matter is self-assembly, i.e. spontaneous organisation of nanometric building blocks into certain structures. This process and the resulting structure depend on the amount of space available for the Brownian motion, the shape of the building blocks, the presence of weak attractive or repulsive interactions between them, as well as external stimuli or fields. By playing with these parameters, one can create many new materials, most of which do not exist in nature and have unprecedented electric, magnetic, optical, and/or mechanical properties and, therefore, are interesting for many applications. The self-assembly of nanometric units is also often seen as a model of similar processes occurring in atomic systems. Several examples of synchrotron studies of the self-assembly process and the resulting structures will be discussed.

Finally, a brief discussion of the effect of the EBS upgrade of the ESRF for nanomaterials and soft matter research will given.

X-ray tomography for Circuit Neuroscience – Towards X-ray Connectomics

Carles Bosch[1], Yuxin Zhang[1], Safe Khan[1], Alexandra Pacureanu[2], <u>Andreas T. Schaefer</u>[1]

Affiliation: [1]Francis Crick Institute, London, UK, [2]ESRF **andreas.schaefer@crick.ac.uk**

The brain is one of the most complex structures known. In order to understand how information is processed in mammalian brains, one needs to combine functional measurements with structural information across scales from cm to nm. In this talk, I will discuss our multi-modal, multiscale approaches, combining functional imaging *in vivo* in mice with different synchrotron X-ray tomography techniques[1,2]. I will illustrate how nano-holotomography can reveal circuit structure at scale, sufficient to describe input-output relationships in a brain area. Moreover, advanced sample preparation approaches[3,4] make it possible to not only prepare samples optimised for X-ray tomography but also to subsequently perform targeted volume electron microscopy with multiple samples. I will conclude by providing an outlook on what the key challenges are for X-ray tomography to delineate neural circuitry at microscopic level[5] and how to scale these approaches up to entire brains.
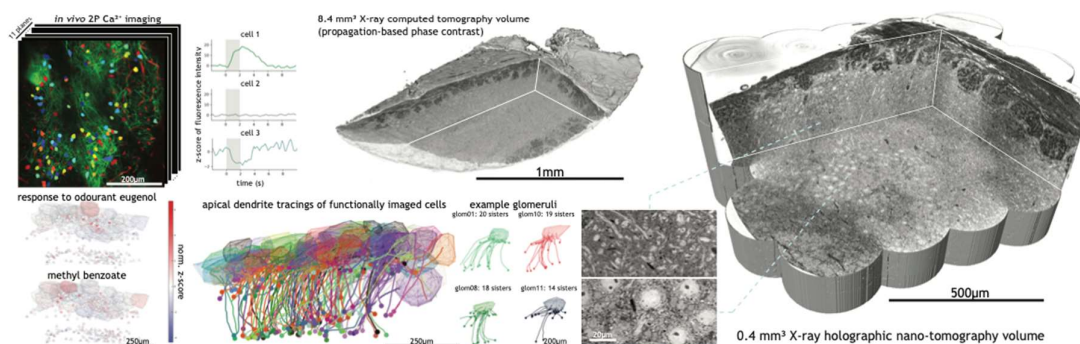
Figure 1: A correlative workflow – combining functional imaging *in vivo* with parallel beam- and holographic synchrotron X-ray nanotomography

References
[1] - Bosch, C., Ackels, T., Pacureanu, A., Zhang, Y., Peddie, C.J., Berning, M., Rzepka, N., Zdora, M.C., Whiteley, I., Storm, M., ,,,, and A.T. Schaefer, Nature Communications 13, 2923. (2022).
[2] - A. Laugros, J. Livingstone, P. Cloetens, A. Pacureanu , A. T. Schaefer. Program No. 144.05. 2023 Neuroscience Meeting Planner. Washington DC: Society for Neuroscience (2023).
[3] - Bosch, C., Lindenau, J., Pacureanu, A., Peddie, C.J., Majkut, M., Douglas, A.C., Carzaniga, R., Rack, A., Collinson, L., Schaefer, A.T., and H. Steigmann. Appl Phys Lett 122, 143701. (2023)
[4] - Zhang, Y., Ackels, T., Pacureanu, A., Zdora, M.-C., Bonnin, A., Schaefer, A.T., and Bosch, C. Frontiers in Cell and Developmental Biology **10**. (2022)
[5] - Bosch, C., Diaz, A., Holler, M., Guizar-Sicairos, M., Aidukas, T., Pacureanu, A., Mueller, E., Peddie, C.J., Collinson, L., Zhang, Y., … A. Diaz, A. Wanner and A.T. Schaefer. bioRxiv 2023.11.16.567403. (2023)

User-Dedicated Microsymposium
UDM 1

7 February 2024

Towards filming macromolecular movies at the ESRF-EBS

UOC Organiser	Adriana Miele
ESRF Organisers	Daniele de Sanctis Montserrat Soler-Lopez
Venue	IBS Seminar room

- ▪ Programme
- ▪ Abstracts of Keynote & User Talks

Towards filming macromolecular movies at the ESRF-EBS

Wednesday, 7th February 2024 - Microsymposium UDM1
Venue: IBS seminar room

Time	Session	Speaker
8:30-8:45	**Registration**	
8:50	Welcome	**Michael Krisch** ESRF Director of Research
	Session I: Chair: Daniele de Sanctis	
09:00	**Keynote: XFEL- and synchrotron-based serial crystallography studies of the membrane-bound proton pump cytochrome c oxidase**	**Gisela Brändén** University of Gothenburg
9:30	**MicroMAX – a beamline with time-resolved macromolecular crystallography capabilities at the MAX IV Laboratory**	**Oskar Aurelius** Lund University
9:50	**The TR-icOS setup at the ESRF: time-resolved microsecond UV-Vis absorption spectroscopy on protein crystals**	**Sylvain Engilberge** ESRF Grenoble
10:10	**Rationale and experimental setup for the use of lower energies in serial micro-crystallography experiments at XAIRA beamline**	**Judith Juanhuix** ALBA synchrotron light Facility
10:30	**Deciphering protein motion at the new ID29 EBS-ESRF**	**Julien Orlans** ESRF Grenoble
10:50	*Coffee break*	
	Session II: Chair: Adriana Miele	
11:10	**Keynote: Envisioning a shared future for serial diffraction from X-rays and electrons**	**Gerhard Hofer** Stockholm University
11:40	**The XFEL Hub at Diamond: Dynamic Structural Biology on Earth**	**Allen Orville** Diamond Light Source
12:00	**Time lapse crystallography using the ultrasonic acoustic levitation diffractometer and its prospects at 4th generation synchrotrons**	**Takashi Tomizaki** Paul Scherrer Institute
12:20 - 13:30	*Lunch*	
	Session III: Chair: Montserrat Soler-Lopez	
13:30	**Keynote: Towards deciphering the structure and dynamics of biological and non-biological molecules using time-resolved serial crystallography at ID29**	**Jose Martin Garcia** IQF-BC CSIC Madrid
14:00	**Decrypting a cryptochrome using time-resolved crystallography and time-resolved spectroscopy; from nanoseconds to seconds.**	**Nicolas Caramello** ESRF Grenoble
14:20	**Serial macromolecular crystallography: developments for high throughput measurements over large parameter spaces.**	**Dominik Oberthur** CFEL - DESY Hamburg

14:40	**Millisecond Cryo-Trapping Through Simplified Time-Resolved Crystallographic Technique**	**Sihyun Sung** EMBL Hamburg
15:00	**A redox switch allows binding of Fe(II) and Fe(III) ions in the cyanobacterial iron binding protein FutA from Prochlorococcus**	**Ivo Tews** University of Southampton
15:20	*Coffee break*	
15:40	**Keynote:** **Time-resolved serial crystallography using photo caged compounds**	**Henrike Müller-Werkmeister** University of Potsdam
16:10	**Ultrafast Dynamics of Biomolecules from X-ray Crystallography Data**	**Ahmad Hosseinizadeh** University of Wisconsin Milwaukee
16:30	**Serial Time-Resolved Crystallography at ESRF ID 29: a User Perspective**	**Tek Malla** University of Wisconsin Milwaukee
16:50	**Keynote:** **A New Approach to Mix-and-Inject Serial Synchrotron Crystallography Resolves the Function of DJ-1**	**Kara Zielinski** Cornell University
17:20	**Concluding remark and general discussion**	
18:00	*End of the Symposium*	

XFEL- and synchrotron-based serial crystallography studies of the membrane-bound proton pump cytochrome *c* oxidase

Gisela Brändén

University of Gothenburg, Sweden, gisela.branden@gu.se

Serial crystallography is a relatively novel method within macromolecular crystallography that allows determination of protein structures at room temperature and enables time-resolved studies of protein dynamics. In my group, we use this method to study the membrane-bound respiratory enzyme cytochrome *c* oxidase, where the ultimate goal is to describe the mechanistic details of proton pumping. I will present our work on microcrystallization of soluble as well as membrane proteins, and also developments within crystal injection methods. Moreover, I will show results from recent static and time-resolved X-ray diffraction experiments on cytochrome *c* oxidase performed at synchrotron- and XFEL facilities, including how the active site dynamics is probed using carbon monoxide as a mimic of the natural substrate oxygen.

MicroMAX – a beamline with time-resolved macromolecular crystallography capabilities at the MAX IV Laboratory

O. Aurelius[1], M. Milas[1], M. Chenchiliyan[1], M. Yazdi-Rizi[1], C. Casadei[1], J. Nan[1], I. Gorgisyan[1], S. Aggarwal, M. Bjelčić[1], S. Benedictsson[1], L. Roslund[1], E. Jagudin[1], M. Eguiraun[1], A. Nardella[1], A. Finke[1], T. Krojer[1], A. Gonzalez[1] & T. Ursby[1]

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With improved tools and capabilities for multi-crystal macromolecular crystallography (MX), the use of experiments under non-cryogenic conditions is increasingly revisited and reimagined. The MAX IV Laboratory, a 4th generation synchrotron source based in Lund, Sweden, has to date operated the BioMAX beamline [1] dedicated towards macromolecular crystallography. BioMAX has offered a range of experimental capabilities, but in particular delivered cryogenic rotation crystallography experiments in a high-throughput manner.

The second MAX IV Laboratory MX beamline, MicroMAX – funded by the Novo Nordisk Foundation, has recently come online and had its first user experiment in 2023. MicroMAX aims to complement BioMAX with microfocus capabilities, as well as to extend functionality for experiments targeting the studies of dynamics of macromolecules. These ambitions include experiment setups for room-temperature crystallography and serial synchrotron crystallography (SSX). Lessons learned from SSX developments at BioMAX [2] are being refined and packaged for both low-dose data collections, as well as more complex pump-probe experiments.

An overview of the MicroMAX beamline project will be presented, including how it will make use of a high data-rate integrating detector, a chopper for tuneable pulsed experiments and the road ahead for extending the beamline capabilities, science cases and its user community.
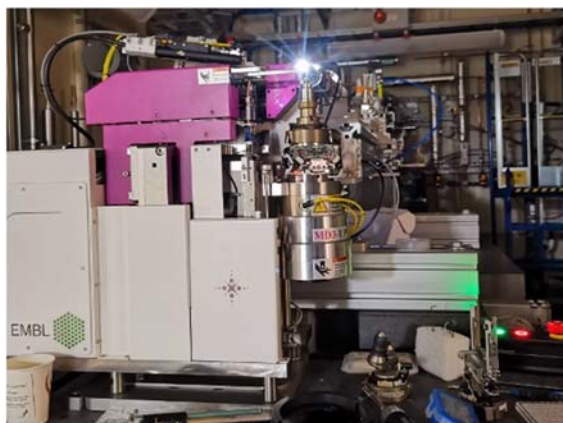

Figure 1: The MicroMAX MD3-UP diffractometer during beamline commissioning.

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The TR-*ic*OS setup at the ESRF: time-resolved microsecond UV-Vis absorption spectroscopy on protein crystals

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The technique of time-resolved macromolecular crystallography (TR-MX) has recently been rejuvenated at synchrotrons, resulting in the design of dedicated beamlines. This should make possible, using pump-probe schemes, the mechanistic study of photoactive proteins and other suitable systems with time resolutions down to microseconds. In order to identify relevant time delays, time-resolved spectroscopic experiments directly performed on protein crystals are often desirable. To this end, we have built an instrument at the *ic*OS Lab (*in crystallo* Optical Spectroscopy laboratory) at the ESRF using reflective focusing objectives with a tuneable nanosecond laser as a pump and a microsecond xenon flash lamp as a probe, which we call the TR-*ic*OS (time-resolved *ic*OS) setup [1]. Using this instrument, one can rapidly record pump-probe spectra from single crystals with time delays ranging from a few microseconds to seconds and beyond. This can be repeated at various laser pulse energies to track the potential presence of artefacts arising from two-photon absorption, which amounts to a power titration of a photoreaction. We have applied this approach to monitor the rise and decay of the M-state in the photocycle of crystallised bacteriorhodopsin and evidenced that the photocycle is increasingly altered with laser pulses of peak fluence greater than 100 mJ/cm^2, providing experimental laser and delay parameters for a successful TR-MX experiment.

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Rationale and experimental setup for the use of lower energies in serial micro-crystallography experiments at XAIRA beamline

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Following the seminal work of Nave and Cowan [1], the use of hard X rays with an energy of 20-30 keV has been considered optimal by the community developing methods for serial and time-resolved crystallography at synchrotron facilities due to the longer mean free path of electrons in the crystal and the relative higher cross-section of the elastic scattering with respect to the other interaction processes with matter [2]. This consideration has been further reinforced with the advent of large pixel array detectors with detective quantum efficiency close to 100% at this energy range [3].

Nevertheless, in a photon hungry technique such as time-resolved serial crystallography, the choice is still not optimal from the point of view of the flux delivered by the undulator source and from the absolute cross-section of elastic scattering by biological material, both much higher at the lower end of the hard X-ray spectrum.

Here we explore the different factors that have led to the choice to exploit the 6-13 keV energy range in serial micro-crystallography experiments. We will also describe how this is implemented at the new BL06-XAIRA microfocus beamline at ALBA synchrotron light source.

XAIRA beamline, which is currently being commissioned, aims to provide a 4-14 keV, stable, high flux beam, focused to 3×1 μm^2 FWHM [4]. The beamline optics include a novel monochromator design combining a cryocooled Si(111) channel-cut and a double multilayer diffracting optics for high stability and high flux, among other developments. The entire end station, including sample environment, cryostream and detector, is enclosed in a helium chamber to reduce X-ray parasitic scattering with air and to improve the signal to noise ratio. The design of the fixed-target serial crystallography setup includes electromagnetic direct drives for fast rastering scans at sub-micron follow up error. The end station is also equipped with a commercial on-axis visualization system together with an undrilled, high-magnification microscope for sample imaging at sub-micron resolution. The current status of the beamline during ongoing beam commissioning is presented here with particular detail on the in-house developed end station and optical elements.

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Deciphering protein motion at the new ID29 EBS-ESRF

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Fourth generation synchrotron sources create new opportunities for expanding the research in structural biology and in protein crystallography in particular. The ESRF Extremely Brilliant Source upgrade programme was completed with the construction of the new ID29, the first world beamline completely dedicated to room temperature experiment and time-resolved macromolecular serial crystallography. The beamline characteristics were designed in order to obtain diffraction data from micrometer sized crystals and achieve a microsecond time resolution. This needed the development of a new class of instrumentation which included a new double chopper timing system, that is able to produce X-ray pulses of 10 microseconds, a new diffractometer, the MD3upSSX, that presents a flexible sample environment, that accommodates fixed target [1-3], viscous injectors [4-6], microfluidics [7] or tape drive [8-11]. The experimental setup is completed with a Jungfrau 4M detector that has been integrated in the ESRF data acquisition pipeline and can be operated up to 1 kHz data acquisition rate.

In this presentation we will report from the first ground-breaking experiments that took place in this initial year of operation of ID29, along with the beamline development roadmap and future plans.

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Envisioning a shared future for serial diffraction from X-rays and electrons

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Recent advances in serial X-ray diffraction (XRD) at ESRF have paved the way for the development of novel approaches in serial electron diffraction (ED) data collection. These advancements have, in turn, led to the exploration of new crystallization methods and data processing strategies, which hold promise for their application back in the realm of synchrotron serial XRD.

This talk focuses on the differences and, more importantly, the similarities between these two methods and the potential advantages of combining forces, speeding up both developments and overcoming individual bottlenecks. By combining the strengths of serial XRD, which probes the electron distribution, with serial ED, which provides electrostatic potential in real space, we open the door to a powerful synergy. The data collected using both methods on the same sample can be harnessed to refine our understanding of their distinctions. This refinement has the potential to illuminate the charge distribution within the sample or offer other insights, such as determining hydrogen positions from sub-micrometer-sized crystals.

The XFEL Hub at Diamond: Dynamic Structural Biology on Earth

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We have developed sample-efficient delivery and reaction initiation strategies that use room temperature microcrystal slurries and serial crystallography methods for time-resolved studies [1, 2]. However, interpreting electron density maps from reaction cycle intermediates can be challenging when mixtures of species are present in the data. Therefore, to help reduce ambiguity we and our collaborators have also pioneered strategies to simultaneously collect time-resolved serial crystallography (tr-SMX/SFX) diffraction data in the forward direction, and X-ray emission spectroscopy (tr-XES) data at ~ 90º, using either XFEL or synchrotron sources. The resulting atomic and electronic structures are fully correlated and have been applied to a range of enzymes [1-8]. For instance, isopenicillin N synthase (IPNS) uses nonheme iron to catalyse the O_2-dependent conversion of its tripeptide substrate δ-(L-α-aminoadipoyl)-L-cysteinyl-D-valine (ACV) into isopenicillin N (IPN, the precursor of all penicillin/cephalosporin β-lactam antibiotics). The unique four electron oxidation reaction leading to the β-lactam bicyclic ring proceeds via two high-valent iron species, an Fe(III)-superoxo and a high-spin Fe(IV)=O oxyferryl species. These enable two sequential C-H bond cleavage steps that each exhibit large kinetic isotope effects (KIE). Our recent tr-SFX and tr-XES studies have characterised the Fe(III)-superoxo species and revealed unexpected, correlated motions throughout the whole protein caused by O_2 binding [3].
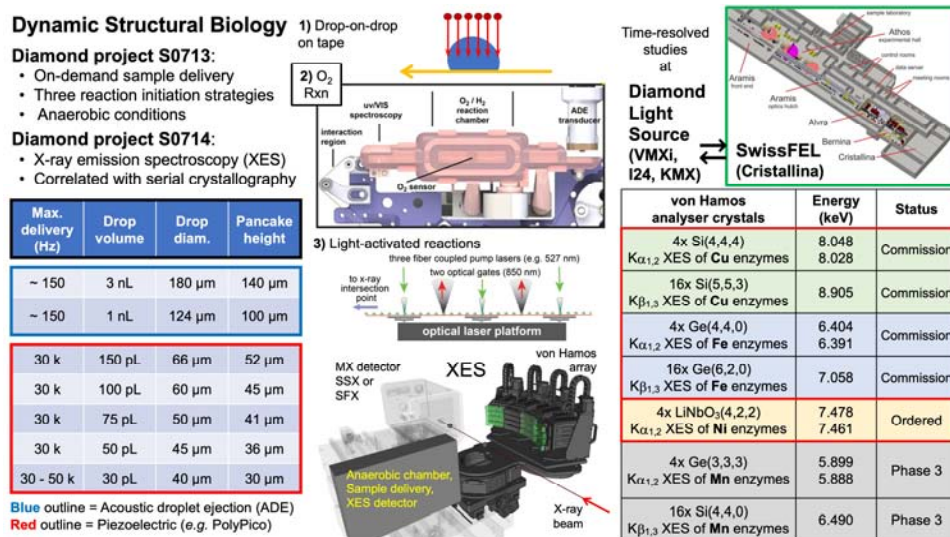
Figure 1: Two projects enable on-demand sample delivery for tr-SMX ± tr-XES.

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Time lapse crystallography using the ultrasonic acoustic levitation diffractometer and its prospects at 4th generation synchrotrons

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The acoustic levitation diffractometer (ALD) can perform diffraction experiments at high sample efficiency and throughput at room temperature using traditionally prepared samples [1]. By taking advantage of room-temperature and liquid environment of the sample, time lapse experiments, aiming at recording molecular movies of slow (1-30 s) reactions, for ligand soaking have been demonstrated [2]. Recently, we introduced thin-film sample holders [3], that are instrumental for establishing a standardised workflow for ALD experiments from the data collection to the data processing. With the new workflow, experiments can be conducted by external users without much specialized assistance. For sample preparation, the positional stability of loaded samples has much improved for achieving high hitrates with uniform triggering by liquid soaking or laser excitation. For data processing, the collected data set from 10-20 runs are first analysed for the best combination of data merging by the hierarchical cluster analysis (HCA) based on the correlation of the structure factors between datasets. Datasets for each time point were subsequently generated by 'partialator' using 'custom split' option in the CrystFEL program suite.

In this talk, the established workflow will be presented with our reference datasets. Preliminary results from end user's projects will also be presented as real-life examples. Reference datasets were also collected on beamline ID29 at the ESRF using the pulsed and high-flux X-ray beam. The results demonstrate the low radiation damage, indicating the feasibility of ID29 and SLS2 for the timelapse measurement.

Figure 1: (left) Snapshot of a droplet on a thin film sample holder. Ligand solution was soaked by a pair of liquid dispensers. $2F$o – Fc electron density maps of apo state of lysozyme (middle) and after 30 seconds of ligand soaking (right).

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Towards deciphering the structure and dynamics of biological and non-biological molecules using time-resolved serial crystallography at ID-29

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Time-resolved serial crystallography (TR-SX), first at X-ray free electron lasers (XFELs) as TR-SFX, and later adapted to synchrotrons as TR-SSX, has become a powerful technique to study reaction mechanisms *in real time*. In my group, we use TR-SX to study the structural and dynamics of biological and non-biological molecules. In my talk, I will present the most recent results obtained for the human NQO1 (hNQO1) enzyme and the MOF BiPF-15. hNQO1 is a FAD-dependent oxidoreductase essential for the antioxidant defense system, stabilization of tumor suppressors, and activation of quinine-based chemotherapeutics, and over-expressed in several tumors. hNQO1 catalyzes the two-electron reduction of quinones to hydroquinones through a very complex mechanism with concomitant negative cooperativity. In an attempt to decipher new structural insights into the flavin reductive half-reaction of the catalytic mechanism of hNQO1, we have carried out room temperature (time-resolved) serial crystallography experiments both at XFELs and at the new ID-29 beamline of the ESRF, coupled to molecular dynamics simulations [1]. Altogether, the results presented here will pave the way for future time-resolved studies, both at XFELs and synchrotrons, of the dynamics of hNQO1 upon binding to NADH as well as during the FAD cofactor reductive half-reaction. This knowledge will allow us to reveal unprecedented structural information of the relevance of the dynamics during the kinetic mechanism that determines the catalytic function of hNQO1.

MOFs are porous crystalline materials made by the joining of molecular building units through strong bonds to form periodic, extended structures with desired topologies. They are investigated in multiple fields including gas separation and gas storage, catalysis, sensing, and drug delivery, among many others. BiFePF-15 is a novel photocatalytically active material developed at the Materials Science Institute of Madrid (ICMM). BiFePF-15 has shown to be active upon irradiation with visible light, and time-resolved spectroscopic studies have already been conducted to investigate the formation of active radical intermediate species. The results demonstrate the involvement of the organic linker in the formation of the intermediates, and suggest a ligand to metal charge transfer process, which is expected to encompass changes in the bond length and angles of the metal atoms involved. We propose to use capabilities at ID-29 to perform pump-probe experiments to investigate these structural changes associated to the light-activated process. This will serve to elucidate the charge transfer mechanism, and their important implications in the photocatalytic process for which this MOF is active.

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Acknowledgements

Decrypting a cryptochrome using time-resolved crystallography and time-resolved spectroscopy; from nanoseconds to seconds.

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Photolyases and cryptochromes belong to the photolyase/cryptochrome superfamily (PCSf), found in all domains of life. Both types of protein possess similar photoactive regions, however, whilst photolyases repair UV induced DNA lesions (namely either cyclobutane pyrimidine dimers or pyrimidine 6-4 pyrimidone photoproducts) the cryptochromes have mostly lost their DNA repair functionality and instead act as light-driven photoreceptors modulating plant growth, circadian rhythms, and magnetoreception[1]. A wide collaboration, led by the team of Manuel Maestre-Reyna (National Taiwan University) involving Lars-Oliver Essen (Universität Marburg), Junpei Yamamoto (Osaka University) and Antoine Royant (IBS, ESRF) have teamed up to decipher the structural changes involved in signal transduction in the animal-like cryptochrome from the green algae *Chlamydomonas reinhardtii* (CraCRY). The chain of events leading to the signalling state happen over a wide timescale, requiring the use of TR-SX (time-resolved serial crystallography) at both synchrotrons and X-ray free electron lasers (XFELs). The fast events following light absorption (ns – 100s of ms) were captured using time-resolved serial femtosecond X ray crystallography (TR-SFX) at the XFEL SACLA in Japan. In a process called photoreduction blue light absorption drives an initial electron transfer from a tyrosine residue to the inactive oxidised flavin adenosine dinucleotide (FAD), resulting in a short-lived FAD intermediate which is then protonated to a long-lived FADH species[2]. Determination of the exact protonation window was accurately pinpointed via time-resolved *in crystallo* spectroscopy (TR-*ic*OS) on a newly built, dedicated setup of the *ic*OS lab at ESRF. The build-up of a tyrosyl radical formed upon the electron transfer then triggers a structural change in the region between the loop carrying the tyrosyl radical and the C-terminal α-helix, ultimately leading to C-terminus unfolding. The latter event could not be fully visualized with the pump-probe methodology used at SACLA, owing to the increasing difficulty of recording long-delay time-points. Thus, the late events leading to the rise of the signalling state (100s of ms to several seconds) were monitored by the time-resolved serial oscillation crystallography (TR-SOX)[3] approach under steady illumination on beamline ID30A3 at the ESRF. Singular value decomposition (SVD) analysis of the resulting difference electron density maps was leveraged to observe the full set of events leading to signal transduction in a flavin-based photoreceptor on a wide timescale ranging from ns to s providing a detailed molecular mechanism for cryptochrome signalling.
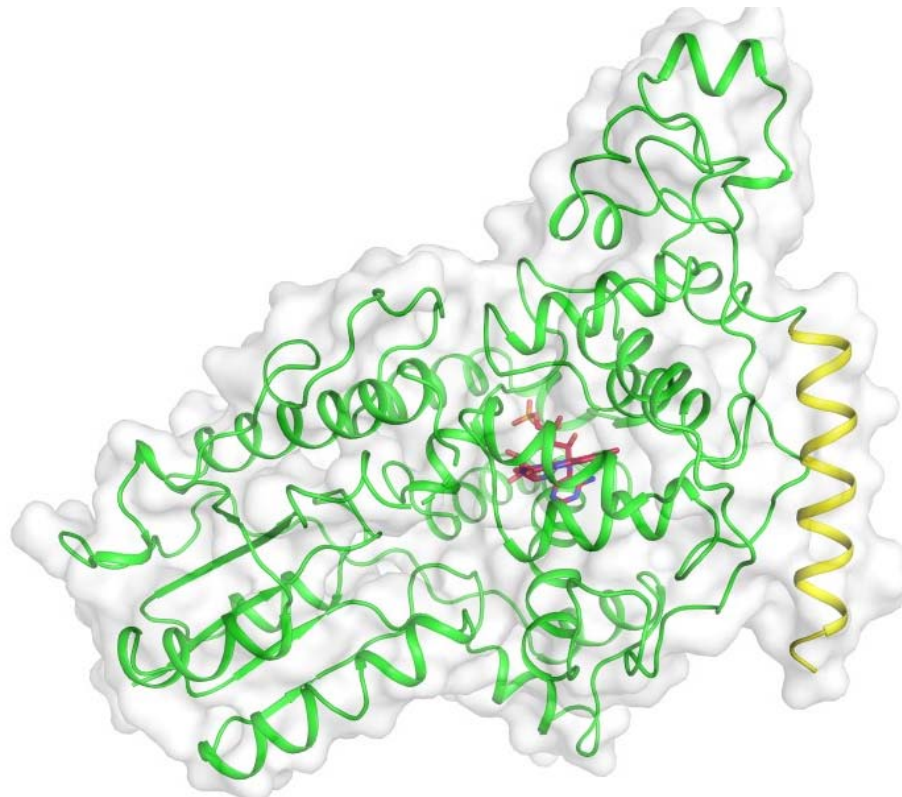
<u>Figure 1</u>: Crystal structure of the CraCRY photoreceptor, with its flavin cofactor (FAD) in red and C-terminus in yellow.

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Serial macromolecular crystallography: developments for high throughput measurements over large parameter spaces.

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Serial macromolecular crystallography (SMX) has emerged as a transformative technique enabling measurements across expansive parameter spaces in structural biology. This talk delves into the evolution of serial crystallography techniques, particularly focusing on developments for time-resolved, pH-responsive, and temperature-controlled experiments and their application in unraveling dynamic structural changes within macromolecules. Highlighting recent results from X-ray Free Electron Laser (XFEL) and synchrotron sources, this presentation explores how serial crystallographyin combination with cutting edge sample delivery and triggering methods can be used to advance our understanding of biological processes. In particular I will talk about how we used the nanofocus beam at EuXFEL to determine the structures of insecticidal proteins[1], how we got a peek into DNA-repair by a photoactive enzyme[2], how we want to take mix-and-inject (SMX) to the next level[3] and how we can utilize the capabilities of ESRF-EBS for this in future.

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Millisecond Cryo-Trapping Through Simplified Time-Resolved Crystallographic Technique

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To understand life on the molecular level, structural biologists study the structure of proteins and other bio-molecules. Many proteins, such as enzymes, don't have a fixed structure – they undergo many structural transformations as they drive reactions with other molecules. Understanding this process step by step is critical to cracking how these proteins work.

Time-resolved serial X-ray crystallography (TR-SSX) captures a protein in action by assembling X-ray snapshots from various reaction timepoints into a molecular movie [1-3]. While TR-SSX demands specialized expertise, a recent collaborative effort by scientists from EMBL Hamburg and the HARBOR has successfully engineered the 'Spitrobot' [4]. This streamlined apparatus provides a more accessible option for non-specialists interested in time-resolved crystallography, facilitating the visualization of catalytic phases by cryo-capturing snapshots of protein behavior during chemical reactions.

Extensive testing of the Spitrobot substantiates its effectiveness in significantly simplifying the monitoring of individual stages within biological reactions. One of the prime examples is Tryptophan synthase (TS), which forms a heterotetrameric assembly comprising TrpA/(TrpB)$_2$/TrpA. In this system, the TrpA product indole is transported to the TrpB subunit via a ~ 25 Å long intermolecular channel to form the final product tryptophan [5,6]. We capture reaction intermediates and conformational changes in the TrpB subunit, showcasing that the Spitrobot allows for insights into catalytic events.
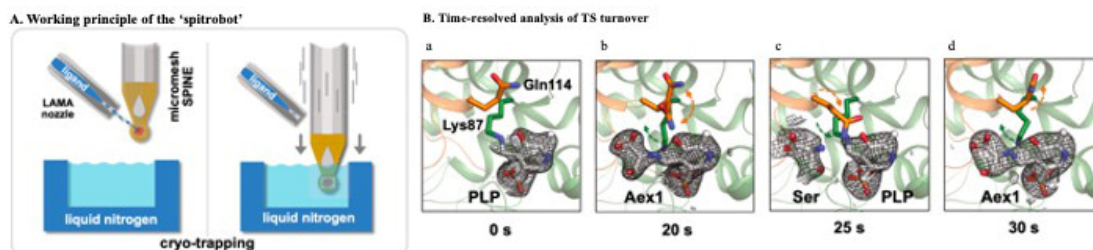
Figure 1: A. Crystals deposited on micro-meshes undergo the LAMA-initiated reaction. Reaction intermediates are vitrified in liquid nitrogen after a specified delay. B. Formation of an external aldimine intermediate (Aex1) is observed at various time points (20 s, 30 s), along with serine binding at 25 s after mixing in the TrpB subunit.

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A redox switch allows binding of Fe(II) and Fe(III) ions in the cyanobacterial iron binding protein FutA from *Prochlorococcus*

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The marine cyanobacterium *Prochlorococcus* is a main contributor to global photosynthesis, whilst being limited by iron availability. Cyanobacterial genomes typically encode two different types of FutA iron binding proteins: periplasmic FutA2 ABC transporter subunits bind Fe(III), while cytosolic FutA1 binds Fe(II). Owing to their small size and their economized genome *Prochlorococcus* ecotypes typically possess a single *futA* gene. How the encoded FutA protein might bind different Fe oxidation states was previously unknown. Here we use structural biology techniques at room temperature to probe the dynamic behavior of FutA. Neutron diffraction confirmed four negatively charged tyrosinates, that together with a neutral water molecule coordinate iron in trigonal bipyramidal geometry. Positioning of the positively charged Arg103 side chain in the second coordination shell yields an overall charge-neutral Fe(III) binding state in structures determined by neutron diffraction and serial femtosecond crystallography. Conventional rotation X-ray crystallography using a home source revealed X-ray induced photoreduction of the iron center with observation of the Fe(II) binding state; here, an additional positioning of the Arg203 side chain in the second coordination shell maintained an overall charge neutral Fe(II) binding site. Dose series using serial synchrotron crystallography and an XFEL X-ray pump-probe approach capture the transition between Fe(III) and Fe(II) states, revealing how Arg203 operates as a switch to accommodate the different iron oxidation states. This switching ability of the *Prochlorococcus* FutA protein may reflect ecological adaptation by genome streamlining and loss of specialized FutA proteins.

Significance. Oceanic primary production by marine cyanobacteria is a main contributor to carbon and nitrogen fixation. *Prochlorococcus* is the most abundant photosynthetic organism on Earth, with an annual carbon fixation comparable to the net global primary production from agriculture. Its remarkable ecological success is based on the ability to thrive in low nutrient waters. To manage iron limitation, *Prochlorococcus* possesses the FutA protein for iron uptake and homeostasis. We reveal a molecular switch in the FutA protein that allows it to accommodate binding of iron in either the Fe(III) or Fe(II) state using structural biology techniques at room temperature and provide a plausible mechanism for iron binding promiscuity.
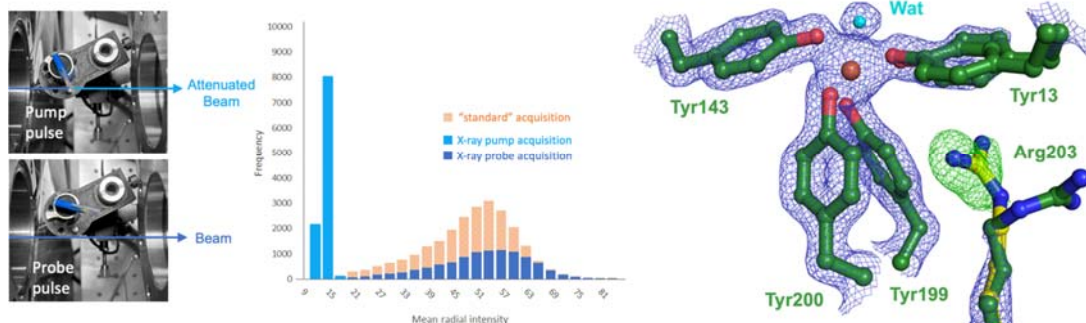
Figure 1: ***The Xray pump probe experiment at SACLA XFEL:*** A fast, self-restoring rotary shutter was mounted upstream of the sample, containing a sapphire wafer. This flipper-attenuator was TTL triggered from a signal generator to reduce the flux with alternating pulses, while two diffraction images corresponding to X-ray pump and X-ray probe were collected on the same crystal. Pump and probe images were separated based on average diffraction intensity (diffraction spots and background) as calculated for each diffraction image and plotted as a histogram against frequency. The X-ray pump (light blue) is distinguished from the X-ray probe (dark blue) by its lower average diffraction intensity. For comparison, a histogram for a standard SFX experiment is shown (salmon). The 2Fo-Fc maps (blue, 1.5 s) and difference density (green, 3 s) after refinement against the SFX structure of the oxidised form (green). The overlay with the reduced state from the home source experiment (yellow) reveals the transition after the pump pulse.

Reference

https://www.biorxiv.org/content/10.1101/2023.05.23.541926v2.

Time-resolved serial crystallography using photo caged compounds

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Time-resolved serial crystallography at synchrotrons and XFELs has paved the way for detailed studies of structural changes during biochemical reactions over many orders of magnitude in time and enabled true multiscale experiments in structural biology.

While several of the pioneering experiments focussed on light-sensitive proteins, including retinal proteins, fluorescent and heme proteins, recent developments target time-resolved serial crystallography (TR-SX) of non-light-sensitive systems.

Two strategies enable studies of proteins, e.g. enzymes without intrinsic chromophore. Mix-and-inject approaches for TR-SX are limited in time-resolution by diffusion. Faster dynamics are accessible when photocaged substrates are used for reaction initiation, in soaked crystals or as co-crystallized ligand. When applying a photocaged substrate in TR-SX studies, as we have demonstrated for the enzyme defluorinase [1,2], the photochemistry of the used photolabile protection group can be altered dramatically in contrast to published characteristics.

Hence, a strong connection between crystallographic and time-resolved spectroscopic work is necessary to optimize reaction initiation and determine accessible timescales within TR-SX studies using photocaged compounds for reaction initiation. We have investigated specifically the influence of pH on photochemistry and found strong influence on reaction yields and absorption characteristics [3]. Depending on the pH, substrate release can either be slowed down or accelerated by several orders of magnitude [4], rendering spectroscopic studies in conjunction with planning the crystallographic experiments even more important.

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Ultrafast Dynamics of Biomolecules from X-ray Crystallography Data

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To date, outstanding efforts have been devoted to accessing structural dynamics of proteins and protein complexes, nonetheless, a precise description of them remains an unsolved problem in biophysics. Response to this question helps to explain many biological phenomena and the creation and work cycle of living organisms. It will also provide revolutionary and new applications and products in other fields such as pharmacology, medicine, biotechnology, industrial chemistry, material science, and so forth. Research on this topic most commonly relies on a few experimental techniques such as NMR spectroscopy, cryo-EM, and X-ray crystallography. However, the level of information extracted by conventional algorithms is severely restricted to a limited number of structures at a few discrete time points. Therefore, access to many intrinsic molecular functions that occur in sub-picosecond timescales remains challenging. To tackle this problem, we have developed and validated a novel data analytic machine learning method [1] capable of extracting detailed structural dynamics information of proteins from experimental data that are corrupted by stochastic artifacts such as noise, timing errors, and data incompleteness. In this presentation, I will review the method and show some results pertaining to the femtosecond structural dynamics of a protein [2].

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Serial Time-Resolved Crystallography at ESRF ID 29: a User Perspective

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Results from our efforts of collecting serial synchrotron data using different sample delivery methods at the new beamline ID29 at the European Synchrotron Radiation Facility (ESRF) are presented. Room temperature data sets on microcrystals of distinct proteins such as the blue and red-light photoreceptors photoactive yellow protein (PYP) and bacterial phytochrome, respectively, as well as on cytochrome-c nitrite reductase (ccNIR) and the SARS CoV-2 main protease 3CLpro were collected using thin foil based fixed targets. The achieved resolution varied from 3.2 Å for the ccNIR to the corner of the detector for PYP. Data quality was excellent throughout resulting in complete datasets for all biological systems. Eventually, using a tape drive system light activated, time-resolved serial crystallography data were collected on bacterial phytochrome microcrystals. Data were good up to 2.3 Å, a resolution usually achieved also at XFELs. The slow reaction in the phytochrome microcrystals was initiated by a photodiode that emits 640 nm light. The illumination time was typically 200 ms. Time-points of 700 ms and 800 ms were collected at two different beamtimes. Both time points show comparable, chemically meaningful signal in difference maps calculated from the collected datasets (Fig. 1). Structural details will be presented and discussed.
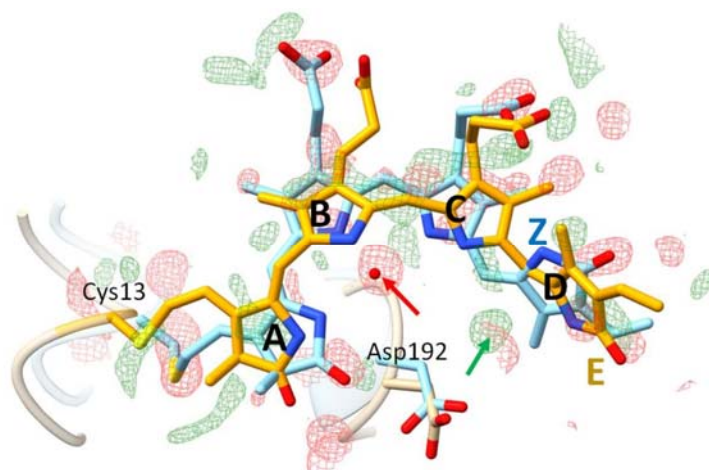
Figure 1: Difference density features near the biliverdin (BV) chromophore 800 ms after photocycle activation. Blue structure: BV in the resting (dark) state, orange structure: BV structure 800 ms after photocycle initiation. BV rings A-D are marked. Ring D is in the Z configuration in the resting state and in the E configuration after 800 ms. Red: negative difference electron density, green: positive difference electron density. Red arrow: the pyrrole water is still absent. Green arrow: putative site for the entry of the pyrrole water.

A New Approach to Mix-and-Inject Serial Synchrotron Crystallography Resolves the Function of DJ-1

Zielinski, K.A.[1], Dolamore, C.[2], Dalton, K.M.[3], Hekstra, D.R.[3,4], Henning, R.[5], Srajer, V.[5], Wilson, M.A.[2], and Pollack, L.[1]

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Time-resolved crystallography is an evolving technique at both X-ray Free Electron Lasers (XFELs) and synchrotrons. Its goal is to capture snapshots of intermediate states of biological reactions to obtain direct structural evidence of reaction mechanisms. Both light-activated and chemically-triggered approaches have been successfully demonstrated, but recent advances in Mix-and-inject Serial Crystallography (MISC) hold particular promise due to its ability to visualize a protein interacting with a small ligand over many time scales. This is achieved by utilizing a flow-focused diffusive mixer to rapidly mix small molecules into a centrally flowing solution of protein crystals to initiate the reaction. Here, we present a new microfluidic device that couples a flow-focused diffusive mixer to a Kapton observation region to perform MISC experiments at synchrotrons. After passing through the mixer, protein crystals undergoing a reaction continue to co-flow with a sheath into the X-ray interaction region to reliably achieve high quality diffraction patterns. By changing the flowrates and the position of the X-ray beam relative to the tip of the mixer, timepoints ranging from ~50 ms – 30 s are reachable. This flow cell was first used at BioCARS at the APS, and datasets were collected in about 1-4 hours, due in part to enhanced information from the polychromatic beam relative to a conventional monochromatic still diffraction pattern. We used this new technology to study DJ-1, an important protein in oxidative stress response. Interestingly, DJ-1's enzymatic function has been heavily disputed, but we directly observed DJ-1 acting on its substrate, methylglyoxal, confirming its role as a glyoxalase rather than a deglycase. Additionally, a few of the intermediate states of the reaction are clear, giving insight into how this important reaction progresses. (Manuscript in preparation)

User-Dedicated Microsymposium UDM 2

7 February 2024

Machine learning and databases in X-ray spectroscopy

UOC Organisers	Guillaume Morard
	Alberto Martinelli
ESRF Organisers	Pieter Glatzel
	Marius Retegan
	Mauro Rovezzi
	Christoph Sahle
Venue	ESRF - Auditorium

- Programme
- Abstracts of Keynote & User Talks

Machine learning and databases in X-ray spectroscopy

Wednesday, 7ᵗʰ February 2024 - ESRF Auditorium		
09:00 – 09:10	Welcome and Introduction	**Vincent Favre-Nicolin**, *ESRF*
	Session I - Chair: V. Favre-Nicolin	
09:10 – 09:50	Machine Learning for X-ray Spectroscopy: Hero or Zero	**Thomas Penfold** *Newcastle University, UK*
09:50 – 10:10	Learning for Sparse Spectral Ptychographic X-Ray Computed Tomography	**Redhouane Boudjehem** *UGA / ILL, France*
10:10 – 10:30	Electronic Structure Calculations Combined With Machine Learning Strategies for the Simulation of RIXS Maps	**Clara L. Silva** *HZDR, Germany*
10:30 – 11:00	*Coffee Break*	
	Session II: Chair: A. Martinelli	
11:00 – 11:40	Machine Learning for Simulating Complex Energy Materials With Non-crystalline Structures	**Nongnuch Artrith** *Utrecht University, Netherlands*
11:40 – 12:00	Exploring the Limits of the Random Forests Algorithm for the Classification of X-Ray Absorption Spectra	**Federico Zecchi** *UGA / ESRF, France*
12:00 – 12:20	Spectrum Classifier for Identifying Sulfur K-edge XANES	**Yuan-Chi Yang** *CEA, France*
12:20 – 13:50	*Lunch Break*	
	Session III – Chair: M. Retegan	
13:50 – 14:30	Structural Decomposition of X-ray Spectra	**Johannes Niskanen** *University of Turku, Finland*
14:30 – 14:50	EXAFS-Precision Metal-Metal Distances From Vibrational Spectra: The Case of Palladium Hydrides	**Aram Bugaev** *PSI, Switzerland*
14:50 – 15:10	Tracking the Ionic Exchange Mechanism in Cu-Exchanged Hydroxyapatites by in Situ XAS: Potential Towards Selective Redox Catalysis	**Sadaf Fatima Jafri** *University of Torino, Italy*
15:10 – 15:40	*Coffee Break*	
	Session IV – Chair: M. Rovezzi	
15:40 – 16:20	Data Formats for XAS Data: Progress Toward Better, Larger, XAS Databases	**Matthew Newville** *University of Chicago, USA*
16:20 – 16:40	*RefXAS*: XAS reference database under DAPHNE4NFDI	**Abhijeet Gaur** *KIT, Germany*
16:40 – 17:00	The SSHADE/FAME Database for X-Ray Absorption Spectroscopy Data	**Denis Testemale and Bernard Schmitt** *UGA / CNRS, France*
17:00 – 17:30	Round Table Discussions	

Machine Learning for X-ray Spectroscopy: Hero or Zero

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X-ray spectroscopy delivers strong impact across the physical and biological sciences by providing end users with highly detailed information about the electronic and geometric structure of matter. To decode this information in challenging cases, e.g., *in operando* catalysts, batteries, and temporally evolving systems [1], advanced theoretical calculations are necessary. The complexity and resource requirements often render these out of reach for end users, and therefore, the data are often not interpreted exhaustively, leaving a wealth of valuable information unexploited.
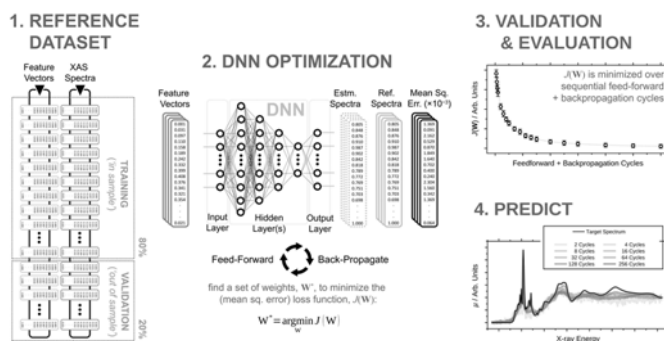
Figure 1: Schematic of the XANESNET workflow discussed in the talk.

In this talk, I will discuss our recent progress applying machine learning to the prediction and interpretation of X-ray spectroscopy [2,3]. This DNN is able to predict X-ray absorption and emission spectra in less than a second with no input beyond geometric information about the local environment of the absorption site. Using the workflow show in Figure 1, we predict peak positions with sub-eV accuracy and peak intensities with errors over an order of magnitude smaller than the spectral variations that the model is engineered to capture.

Throughout the performance of the network will be exemplified with examples and applications. In additions, besides performance, I will also discuss how the network is able to incorporate electronic information, assess uncertainty and interpret predictions [4]. Finally, I will highlight areas on which future developments should focus.

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Learning for sparse spectral ptychographic x-ray computed tomography

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X-ray nanotomography is a well-established technique with many applications in material science and biology. The spatial resolution of classical CT can be enhanced when using ptychographic projections [1] measured at different angles to reconstruct a 3D volume.

X-ray Ptychography [2][3] is a coherent diffraction imaging technique based on the acquisition of multiple diffraction patterns obtained through the illumination of the sample at different partially overlapping probe positions. Information about the sample's transmittivity is obtained by an iterative reconstruction, yielding the imaginary and real part of the complex refractive index, δ and β. Repeating the tomographic acquisitions at different energies allows to add spectral capabilities, and gain information about the localization of a chosen element of interest. The invaluable advantage of this technique is its high spatial resolution in the range of some tens of nanometers for large sample volumes. However, the acquisition of ptychographic tomogram can take half a day or more, depending on the size of the sample, the number of projections and the exposure time. Reducing the number of projections and/or the exposure time would reduce the acquisition time, but these solutions will directly affect the resolution and the reconstructed tomogram will be noisy. This problem can be overcome with help of deep learning. Recently, a Generative Adversarial Network (GAN) [4] called TomoGAN [5][6] was proposed to improve the quality of images obtained by high-resolution tomography. TomoGAN model can be trained with limited data, performs well with high-resolution datasets, generates greatly improved reconstructions of low-dose and noisy data, and is very resilient to overfitting. Previous works demonstrated that the number of projections required can be reduced by a factor of at least 8 while keeping high quality of the reconstructed images. We will show here, how this technique can be applied to the case of spectral tomography, as an example, we will take 2 tomograms of the same sample recorded at two different energies, taking advantage of the similarity of the tomograms. By training the networks on one complete high-resolution tomographic dataset at a given energy, we are capable to retrieve images from tomographic dataset at another energy with much fewer projections than what would be necessary for the retrieved good-quality images using standard algorithms.

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Electronic structure calculations combined with machine learning strategies for the simulation of RIXS maps

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Extracting correlations between X-ray spectroscopic data, the local environment surrounding the absorbing atom, and its electronic structure is not straight-forward for structurally complex systems. In particular, for the K pre-edge of 3d transition metals, many factors affect the spectral features, including the local structure, oxidation state, and nature of ligands. 1s2p resonant inelastic X-ray scattering (RIXS) calculations based on the crystal field multiplet theory provide valuable insights into the interpretation of the K pre-edge of Fe systems [1]. However, when the local environment is unknown beforehand, the calculation procedure to model an experimental spectrum requires a large number of trials using different sets of parameters. In this work, the 1s2p RIXS technique was used to study the local environment and electronic structure of Fe in metal-organic thin films grown by atomic/molecular layer deposition [2]. The RIXS measurements were performed at the beamline ID26 of the European Synchrotron Radiation Facility (ESRF). From the theoretical perspective, as the coordination and local structure of Fe in the thin films were unknown, the insights into the interpretation of the measured RIXS maps were the result of a systematic investigation of a large number of multiplet-calculated spectra. To optimize the workflow of the data analysis, we propose a strategy using machine learning techniques to quantitatively predict spectral parameters for the calculation of the RIXS maps. The best agreement between data and calculations is shown in Fig. 1. The results of our integrated experimental and theoretical study with the machine learning strategy may serve as a starting point for further investigations aiming to maximize the amount of information that can be extracted from the RIXS experimental spectra.

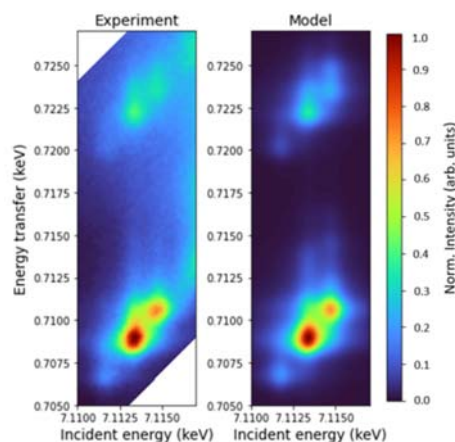Figure 1: Experimental *versus* calculated 1s2p RIXS maps at the Fe K pre-edge.

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Machine Learning for Simulating Complex Energy Materials with Non-Crystalline Structures

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Many materials with applications in energy, e.g., batteries, are non-crystalline, exhibiting amorphous structures, chemical disorder, and complex compositions. This complexity makes direct modeling with first principles methods challenging. To address this challenge, we developed accelerated sampling strategies based on machine learning interatomic potentials, genetic algorithms, and molecular-dynamics simulations [1]. Here, I will discuss the methodology and its applications to amorphous battery materials. We constructed the phase diagram of amorphous LiSi alloys, which are prospective anode materials for lithium-ion batteries [2]. Additionally, we mapped the composition and structure space of amorphous lithium thiophosphate (LPS) solid electrolytes [3-5]. The thermodynamic stability and ionic conductivity of the non-crystalline phases were correlated with local structural motifs, leading to the identification of structure-composition-conductivity relationships that can be used for materials optimization and design. X-ray absorption spectroscopy (XAS) characterizes materials, revealing details of the absorber atom's local chemistry. Our work created an S/P K-edge XAS spectra database for LPS materials using structures from [3]. This study presents the initial atomic-scale insights into the oxidative degradation of LPS electrolytes, guiding macroscopic reactions via microstructural engineering and enhancing sulfide electrolyte design.
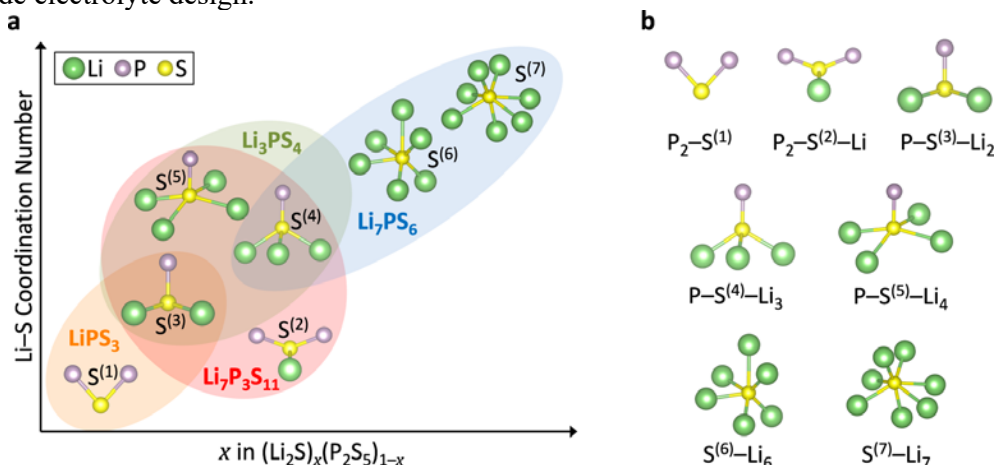
Figure 1: Schematic illustration [4] of the local coordination of S atoms with Li and P atoms in selected $(Li_2S)_x(P_2S_5)1–x$ crystalline structures. Li: green; S: yellow; P: purple. $LiPS_3$: orange region; $Li_7P_3S_{11}$: red region; Li_3PS_4: green region; Li_7PS_6: blue region.

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https://doi.org/10.48550/arXiv.2310.00794

Exploring the limits of the random forest algorithm for the classification of X-ray absorption spectra

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X-ray absorption spectroscopy gives access to a wealth of information regarding the local structure and electronic properties of materials. However, data analysis is significantly more time-consuming than the acquisition and initial data reduction. Decoding the information relies on comparison with similar compounds for which the spectrum–property mapping is already established, a task that is very often performed by visual inspection.

Machine learning (ML) is revolutionizing many fields with its ability to extract and learn patterns in big data without having to provide additional prior information other than the data itself. ML models give access to instantaneous predictions of properties and observables, which makes them particularly attractive for performing autonomous experimental acquisitions or real-time analysis of the measured data.

Current ML applications for X-ray spectroscopy mainly use neural networks (NN), which require extensive computational datasets as training data.[1,2] These are very time-consuming to build and are often linked to large-scale computing facilities access. Alternatively, one can use tailor-made ML models that are less data-hungry and can be trained significantly faster. One such ML algorithm is the random forests, which has already shown promising applications for analyzing visible and infrared spectra.[3]

In the present contribution, we will present the application of the random forests algorithm to identify the coordination environment of iron in a given compound from the corresponding K-edge X-ray absorption spectrum. As we train the model using theoretical data, but we use it to infer properties on measured spectra, we analyze the different sources of errors that limit the quality of the prediction, such as spectral shift, normalization, and noise level. In addition, we explore the use of SMOTE to tackle the class imbalance, a common issue in such datasets as most materials in nature tend to adopt a small set of specific coordination environments.
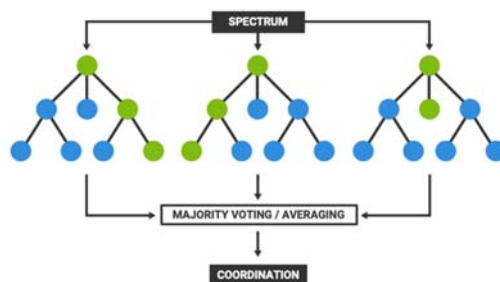
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Spectrum classifier for identifying Sulfur K-edge XANES

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The aim of the topic was quantifying the concentration and identifying the species of polysulfides (Li_2S_x, x = 2~8) within solid polymer electrolytes by sulfur K-edge HERFD-XANES measurement. Because of the strong self-absorption of Sulfur and to avoid beam damage, 100 fast HERFD-XANES at different spots within each sample were measured to acquire enough statistics to resolve the fine structure. Such measurement condition requires ultra-precise sample alignment which is often difficult to achieve. Moreover, polysulfides are prone to contamination, and the sign of contamination can only be identified after merging 100 rough HERFD-XANES. As a result, users often lose valuable beamtime on measuring misaligned or contaminated samples without awareness. To assist users in getting the most out of beamtimes, the sample spatial concentration visualizer equipped with the random forest model-based spectrum classifier is developed. The tool visualizes the coordination and classifies the sulfur species at different measuring spots, and shows the concentration contour profile of samples. In Fig. 1a, the measuring spots on the right-hand side show very low concentration, a sign of misalignment. In Fig. 1b, the tool classifies the measured spectrum at each spot into classes and shows the concentration heterogeneity of the sample. As a result, the tool can help users achieve basic on-the-fly data analysis and decision-making during beamtime. Once the sign of misalignment (low number of effective measuring spots) and sample contamination is detected, the tool can send a warning to users and provide users with visualized sample conditions, so users can realign the samples and make decisions on changing samples in time. For further data treatment, the tool also helps to enhance the signal-to-noise ratio by removing misaligned measuring points when merging the spectrum. The uncorrected and corrected spectra are shown in Fig. 1c.
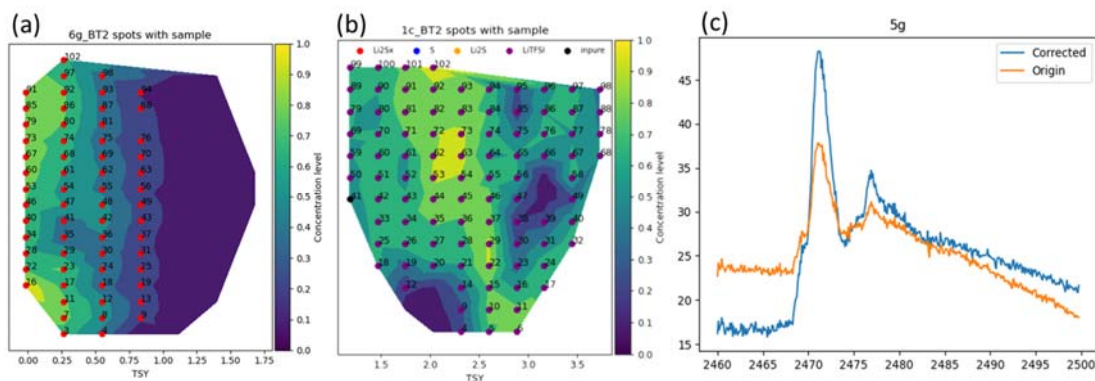
Figure 1: (a) The example of visualizing the misaligned sample. (b) The example of spectrum classification and concentration profile visualization. (c) The comparison of the uncorrected and corrected spectra.

Machine-learning-based decomposition for X-ray spectroscopy

J. Niskanen

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A liquid or an amorphous system allows for the movement of interacting molecules or atoms, which leads to a broad distribution of possible configurations. These individual configurations have been computationally observed to have significantly different X-ray spectra, only the ensemble mean of which predicting the experimentally observed spectrum. Even though interpretation of these spectra may not always be straightforward, they are a widely used probe for structural information. We approach the problem stepwise, first identifying structural degrees of freedom with spectral sensitivity, and second carrying out a structural reconstruction in terms of them.

We will present our ongoing work with interpretation of X-ray spectra (such as XPS, XAS and XES) in terms of underlying atomistic structure. We study simulated data and present a machine-learning-based algorithm for dimensionality reduction in the structural space so that explained spectral variance is maximized [1]. With this algorithm it is possible to find structural degrees of freedom with most spectral dependence and filter the insignificant degrees of freedom out. We then proceed with a case study where the algorithm is used to transform the inverse problem from spectra to structure into a low-dimensional, easier solvable, one [2]. We find that ensemble mean distances of from the active Ge site can be reconstructed from the ensemble mean Ge K beta emission spectrum of amorphous GeO2 at elevated pressures. The contribution also covers some ongoing work with molecular liquids [3].

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EXAFS-precision metal-metal distances from vibrational spectra: The case of palladium hydrides

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Vibrational spectroscopies are widespread techniques for operando characterization of heterogeneous catalysts. Being sensitive to the vibrational structure of the adsorbed molecules, they are often used to identify chemisorption sites, reaction intermediates etc. At the other hand, evolution of the structural parameters of the catalyst itself, which often affects the catalyst's performance, often require bulk sensitive techniques, such as X-ray absorption spectroscopy (XAS), application of which is troublesome due to the demand for synchrotron radiation sources. In the last decade, Machine learning (ML) was demonstrated to enhance significantly the amount of information that can be extracted from spectroscopic data [1-3]. In this work, we demonstrate how vibrational spectra can be used as a source of quantitative structural information by applying ML algorithms. Focusing on the palladium hydride phase formation in the supported palladium nanoparticles (Pd/Al_2O_3), which can occur during numerous industrially relevant hydrogenation reactions, we collected, under exactly identical conditions, XAS and diffusive reflectance infrared Fourier-transformed spectroscopy (DRIFTS) data in a wide range of temperatures and partial hydrogen pressures in presence of CO as a probe molecule. Then, ML algorithm was trained on the dataset made of experimental XAS and DRIFTS data, showing that it is possible to predict structural parameters of Pd nanoparticles from DRIFTS spectra of the adsorbed CO and revealing perspective descriptors of both structural parameters of palladium nanoparticles and DRIFTS data. The experimental results were supported by the density functional theory (DFT) calculations modelling the change in vibrational modes upon the formation of hydride phase. In summary, ML algorithm, trained on a vast dataset of EXAFS and DRIFTS spectra, is now capable to predict Pd-Pd distances from IR data with the precision comparable to that of EXAFS technique.
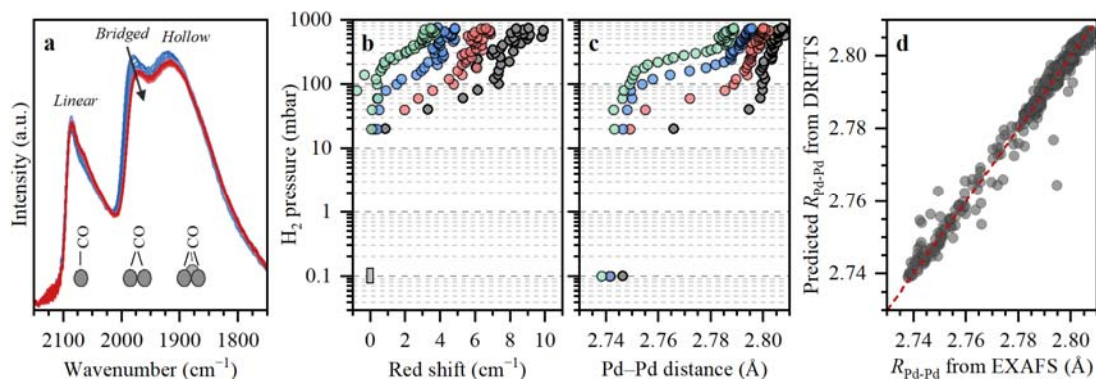
Figure 1: (a) Evolution of DRIFTS spectra in the region of CO vibration upon increase of the H_2 partial pressure (from blue to red) at 30 °C. (b) Red shift observed for bridge CO vibration upon increase of the H_2 partial pressure at 30 (black), 50 (red), 70 (blue) and 90 (green) °C. (c) Pd–Pd distance from EXAFS data measured under identical conditions. (d) Pd–Pd distance predicted from DRIFTS based on the absolute positions of three CO peaks versus true distance obtained from EXAFS.

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Tracking the ionic exchange mechanism in Cu-exchanged Hydroxyapatites by in situ XAS: potential towards selective redox catalysis

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Investigation of the catalytic activity and elucidation of the molecular mechanisms that govern the reactivity of heterogenous catalysis pose big challenges for data analysis with very large sets of spectra. With the advancements in efficient designing of catalysts, significant progress was also made to improve spectroscopic characterization techniques such as X-ray Absorption Spectroscopy (XAS) coupled with theoretical and computational data analysis tools. In last decade, unsupervised and supervised machine learning approaches were developed for extracting the hidden parameters revealing the structure-property dependence for instance, contributions of different metal sites, quantitative structural information about the local environment of active species during catalysis [1].

In this talk, I will present in situ XAS results on copper-exchanged Hydroxyapatite (**Cu-HA**) which is a green catalyst [2]. Hydroxyapatites (**HA**, $Ca_{10}(PO_4)_6(OH)_2$), commonly known as calcium phosphate, are versatile materials that can maintain their structural entity upon substituting any of their basic units by ionic species possessing similar characteristics [3]. The ion exchange mechanism involving substitution of the Ca^{2+} by Cu^{2+} ions and nature of Cu-substituents in **HA** at the molecular level need to be fully understood [4]. Element specific K-edge in situ XAS spectra recorded at BM31(ESRF) on **Cu-HA** samples with a Cu loading of 2-7 wt. % and high surface area. The experimental Cu K-edge XAS coupled with computational tools provided a full characterization of Cu-HA in terms of Cu oxidation state and coordination environment, under model conditions designed to explore the potential of these materials towards selective oxidation catalysis. XANES Multivariate Curve Resolution (MCR) - an unsupervised machine learning tool, in combination with PyFitit software, facilitated in extracting the underlying chemical information about the number and the nature of the pure Cu species involved in the catalysis (fig. 1).
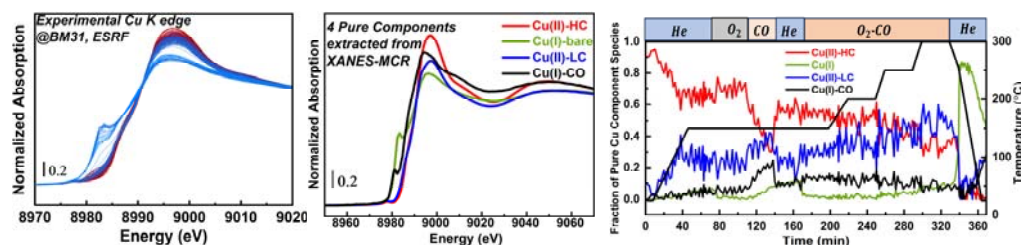
Figure 1: Experimental in situ XAS spectra recorded at Cu K edge **(left)**, four pure component of Cu species extracted from XANES-MCR **(middle)** and their corresponding concentration profile **(right)**.

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Data Formats for XAS Data: progress toward better, larger, XAS Databases

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XAS data gives unique information about the chemical state of materials. High-quality XAS data requires well-prepared samples and access to valuable synchrotron beamlines or state-of-the-art laboratory sources, XAS data is a rare and valuable commodity. Well-maintained databases of XAS spectra on both standard reference materials and samples then become important for the synchrotron and scientific communities, both for individual researchers and for automated machine-learning methods. Enabling the automated use of spectral libraries requires curated and documented formats and metadata fields for the spectral data. I will present existing XAS spectral libraries and formats, and report on progress from a Working Group from the XAFS community towards standardizing metadata and defining specifications for both plain text and NeXuS/HDF5 formats for XAS data.

RefXAS: XAS reference database under DAPHNE4NFDI

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X-ray absorption spectroscopy (XAS) is a crucial method for analysing solid materials, including amorphous materials, and is widely used in various fields. In XAS research, data are often evaluated by comparing them to previously measured or calculated reference spectra. Automatic, also on the fly, data processing requires a repository with high quality reference data, including metadata, from reliable sources. This sets the high requirements concerning both spectral quality and documentation of the measurements, i.e., metadata [1]. Under DAPHNE4NFDI, we have been working on to set up a XAS reference database, *RefXAS*, including raw and processed data with an interface developed for uploading and evaluating the data. With the defined metadata/data fields and quality criteria, a prototype database is running where different features of the database are tested. After going through available options an online data submission process for the users has been developed. The format/structure of metadata for the uploaded data displayed on the interface and available for users to be downloaded has been finalized. XAS spectra from different beamlines/synchrotron facilities and laboratory facilities having distinct data/file formats have been tested for uploading at the developed interface. A human verification procedure for the uploaded data will be implemented for checking and validating the data. One of the application of such curated database is that it would be possible to compare the data for identical samples from different facilities and hence the effect of different parameters of an instrument on the data quality can be studied. In this talk, the importance of defined metadata fields and formulation of quality criteria for the data uploaded at the XAS database will be discussed. The developing features of running prototype of the database will be shown.
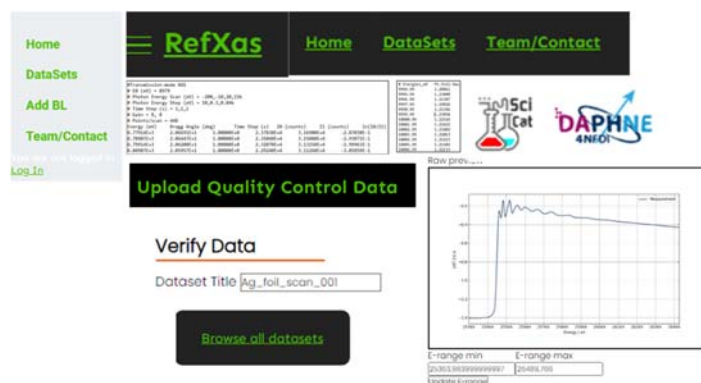
Figure 1: A snapshot of *RefXAS* database website displaying different features

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The SSHADE/FAME database for x-ray absorption spectroscopy data

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The French X-ray spectroscopy beamlines at the ESRF, FAME (BM30) and FAME-UHD (BM16) have created the SSHADE/FAME database (https://www.sshade.eu/db/fame), in order to provide X-ray absorption spectra linked to a detailed sample description and validated quality, in order to improve their access and reusability by the users community. The database currently contains 603 spectra and is constantly feeded with new spectra. It is hosted within the SSHADE infrastructure (Solid Spectroscopy Hosting Architecture of Databases and Expertise, https://www.sshade.eu), an European funded project (H2020 european programs "Europlanet 2020 RI" and "Europlanet 2024 RI"). It is comprised of multiple databases containing spectral data from many different types of materials (minerals, molecular solids, meteorites, organic materials, liquids, etc.) as well as calculated spectra, and covering the whole electromagnetic spectrum from gamma rays to radio wavelengths. This common infrastructure provides an extended and standardized sample metadata model, SSDM (Solid Spectroscopy Data Model), which also enables efficient search strategies. SSHADE's interface, with search/view/download capabilities and DOI referencing of data, is open to users since February 2018.

After a presentation of the SSHADE/FAME database, the import mechanism and search tools will be described, along with some examples of its interface and use for FAME XAS data. The perspectives for future developments will also be discussed: simplified data model and accessibility.

User-Dedicated Microsymposium
UDM 3

7 February 2024

The complementary use of diffuse and inelastic X-ray scattering

UOC Organiser	Beatrice Ruta
ESRF Organisers	Alexei Bosak
	Daniel Chaney
Non-ESRF Organiser	Aleksandra Chumakova
Venue	MD-1-21

- Programme
- Abstracts of Keynote & User Talks

The complementary use of diffuse and inelastic X-ray scattering

Programme

Wednesday, 7th February 2023 - Microsymposium UDM3		
Session I		
08:15 – 08:45	Registration in the ESRF Central Building	
08:55 – 09:00	Introduction to the microsymposium UDM3	
09:00 – 09:30 Keynote 1	**Phonon anomalies in Kagome metals**	**Dr Santiago Blanco-Canosa** *Donostia International Physics Center, Spain*
09:30 – 09:50 Contributed 1	**Charge order and diffuse scattering at high pressures**	**Dr Björn Wehinger** *ESRF, France*
09:50 – 10:10 Contributed 2	**Pressure and disorder quenching of the charge density wave in ZrTe$_3$**	**Dr Moritz Hoesch** *DESY, Germany*
10:10 – 10:30 Contributed 3	**Charge density waves and soft phonon evolution in the superconductor BaNi$_2$(As$_{1-x}$P$_x$)$_2$**	**Tom Lacmann** *Karlsruhe Institute of Technology, Germany*
Coffee break (10:30 – 11:00)		
Session II		
11:00 – 11:30 Keynote 2	**Insights into the local structure of materials from single crystal diffuse scattering**	**Prof Arkadiy Simonov** ETH Zürich, Switzerland
11:30 – 11:50 Contributed 4	**Disorder engineering for symmetry lowering in Prussian Blue analogues (PBAs)**	**Yevheniia Kholina** ETH Zürich, Switzerland
11:50 – 12:10 Contributed 5	**Local correlations and lattice dynamics in advanced nuclear fuels**	**Dr Daniel Chaney** *ESRF, France*
12:10 – 12:30 Contributed 6	**Probing the interplay of static disorder with lattice dynamics using inelastic X-ray and neutron scattering**	**Dr Johnathan Bulled** *University of Oxford, UK*
Lunch Break (12:30 – 14:00)		

Session III		
14:00 – 14:20	**ID28 tandem beamline – Current status and upcoming upgrade**	**Dr Alexei Bosak** *ESRF, France*
14:20 – 14:50 Keynote 3	**Supercell lattice dynamical calculations to predict thermal diffuse scattering in materials with correlated disorder**	**Prof Ella Schmidt** University of Bremen, Germany
14:50 – 15:10 Contributed 7	**Thermal diffuse scattering of framework materials: a coarse-grained approach**	**Quentin Gueroult** *University of Oxford, UK*
15:10 – 15:30 Contributed 8	**Phonon dispersion relations of novel phases in 1D nanosystems. Case study: wurtzite InP nanowires**	**Dr Jorge Serrano** *University of Valladolid, Spain*
15:30 – 15:50 Contributed 9	**Evolution of charge order from underdoped to extremely overdoped region of the cuprate superconductor $La_{2-x}Ca_xCuO_4$**	**Dr Sanjna Hameed** *Max Planck Institute for Solid State Research, Germany*
15:50 – 16:00	Closing remarks	

Diffuse and inelastic x-ray scattering in kagome metals

Santiago Blanco Canosa[1,*], Artem Korshunov[2], Haoyu Hu[1], David Subires[1], Jiang Yi[3], Dumitru Calugaru[4], Xiaolong Feng[8], Anil Rajapitamahuni[5], Changjiang Yi[8], Subhajit Roychowdhury[8], Maia Vergniory[1], Joerg Strempfer[6], Chandra Shekhar[8], Elio Vescovo[5], Dmitry Chernyshov[7], **Brenden R. Ortiz, Stephen**[9], **D. Wilson**[9], Ayman Said[6], Alexei Bosak[2], Claudia Felser[8], Andrei Bernevig[1,4]

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5. National Synchrotron Light Source II, Brookhaven National Laboratory, Brookhaven, USA
6. Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois, USA
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The long range electronic modulations recently discovered in the geometrically frustrated kagome lattice have opened new avenues to explore the effect of correlations in materials with topological electron flat bands [1]. In this talk, I will present diffuse scattering and IXS data in several kagome metals that allow a comprehensive study their phase transitions. I will focus on the recently discovered multiple-**q** charge modulations in $(Cs,Rb)V_3Sb_5$ [2], $FeGe$ [3]and ScV_6Sn_6 [4] and explain how their dynamics follow either an order-disorder scenario common in first order phase transformations or a phonon softening characteristic of a second order phase transition. Furthermore, I will show the potential of diffuse scattering to identify primary order parameters and its coupling/competition to secondary orders in the study of multiple-**q** charge density waves in materials hosting correlated flat phonon-topological flat electron physics.
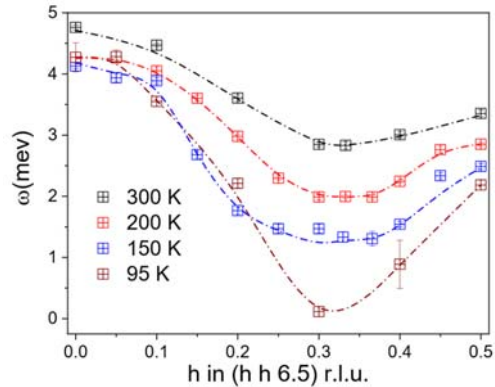
Figure 1: Momentum dependence of the 1/3 1/3 13/2 phonon frequency at selected temperatures, highlighting the large momentum softening in ScV_6Sn_6.

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Charge order and diffuse scattering at high pressures

B. Wehinger[1]

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I will present diffuse scattering in quantum materials where localized spins are arranged on kagomé lattices and electronic correlations are enhanced due to ensuing electronic interactions. In the prototypical kagomé superconductor $LaRu_3Si_2$ [1] charge orders above room temperature resulting in pronounced superstructure reflections and diffuse scattering. I will show how pressure acts as clean tuning parameter for the underlying correlations with intriguing changes on the diffuse scattering. High-precision measurements of diffuse scattering at high pressures are now possible at ESRF and in the second part of my talk I will show how quantitative analysis is possible with and without complementary inelastic x-ray scattering experiments [2].

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Pressure and Disorder Quenching of the Charge Density Wave in ZrTe₃

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The prototypical weak-coupling charge density wave (CDW) in ZrTe₃ can be quenched by either hydrostatic pressure [1] or disorder [2]. The pure material, for pressures up to 5 GPa shows CDW transitiosn at temperatures between 60 and 100 K. The disorder can be of minute degree by chemical substitution of a few percent of Se against Te and in this case no CDW features are observable by diffraction or transport. In both cases bulk superconductivity emerges, which is not supported in pure ZrTe₃. A Raman study assigns the quenching with pressure to disorder in the very soft material, too [3], while a x-ray diffraction study, conducted under similar hydrostatic pressure conditions, finds no signature of disorder with pressure and invokes an misbalancing of Fermi surface nesting as responsible for quenching with pressure [4].

Thus the origin of CDW quenching with pressure remains unresolved, while the subtle disorder effect of ZrTe₂.₉₇Se₀.₀₃ is uncontroversially responsible for the quenching, with the fascinating consequence of having a disordered one-dimensional superconducting state.

In this study we set out to clarify the similarity and dissimilarity of CDW quenching in ZrTe₂.₉₇Se₀.₀₃ at ambient pressure on one hand and in pure ZrTe₃ at hydrostatic pressures up to 6 GPa on the other. Diffuse scattering in ZrTe₂.₉₇Se₀.₀₃ shows an intriguing system of either quasistatic ordering or soft-phonon regions across almost all of x-ray scattering space, including regions where pure ZrTe₃ at low pressure shows the characteristic superstructure peaks. These diffuse scattering features remain, however, broad and weakly correlated down to very low temperatures (12 K) in the disordered material. Inelastic X-ray Scattering (IXS) shows a slight Kohn anomaly only, along with a strong quasielastic peak. The diffuse scattering thus originates from quasi-static order. The situation is entirely different in pure ZrTe₃ beyond the quenching pressure of 5 GPa. Here, the Kohn anomaly is of giant nature, thus leading to the freezing of the known soft phonon mode an even though superstructure diffraction is no longer detectable with reasonable contrast, the phonon effects are similar at the pressure beyond 5 GPa as they are in the CDW regime below.

We present the observed data of both diffuse x-ray scattering and IXS and discuss potential scenarios for the two kinds of CDW quenching by highlighting tbe observed similarities and differences.

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Insights into the local structure of materials from single crystal diffuse scattering

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In this presentation, I will discuss the methodology of diffuse scattering analysis and its applications for studying local structure of materials with chemical disorder. I will present a few peculiar examples in which local structure breaks the average crystal symmetry and gives rise to the average-symmetry-prohibited properties, like birefringence and ferroelectricity.

Disorder engineering for symmetry lowering in Prussian Blue analogues (PBAs)

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A simple consequence of Neumann's principle, that certain properties can exist in crystals with a certain symmetry. For example, ferroelectricity can only emerge in crystals with polar space groups. As a result, a lot of materials engineering is focused on designing particular symmetries, which allow the properties of interest. In oxide perovskites as well as their molecular analogues, control of crystal symmetry is typically achieved by octahedral tilts and cation ordering [1].

In this work we show an alternative way of symmetry lowering, using disorder. We focus on Mn[Co] Prussian Blue Analogue, disordered molecular analogue of perovskite with the chemical composition $Mn[Co(CN)6]2/3$. These crystals have 1/3 of $Co[CN]6$ sites vacant. The structure of such PBAs is believed to be cubic with space group $Fm\bar{3}m$ at ambient conditions. However, the optical measurements indicate that the crystal is twinned and an actual structure has tetragonal symmetry or lower.

We collect single-crystal x-ray diffuse scattering from untwined crystal to probe the local structure and quantitatively characterize defect distribution, using 3D-ΔPDF analysis. The symmetry of the local structure is reduced to tetragonal 4/mmm by local vacancies ordering (Fig.1). The vacancies have stronger correlation along the special direction of tetragonal lattice. Such asymmetry is formed because the crystal is growing in this direction. This means that in such crystals, symmetry can be lowered by simply choosing a specific direction of the crystal growth.
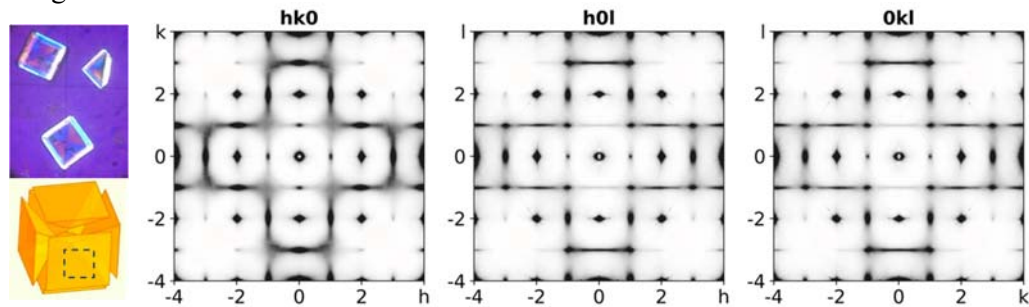
Figure 1: Tree projections of experimental diffuse scattering from untwined Mn[Co] Prussian Blue analogue..

We believe this result can be applied to other disordered crystalline materials (such as host-guest structures [2]) and be an effective way to lower the symmetry for properties design.

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Local correlations and lattice dynamics in advanced nuclear fuels

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The international fission reactor fleet may be broadly categorised as being either power or research reactors. Both have and will continue to play a pivotal role in addressing key challenges of our society. It is widely accepted that in many countries the green energy transition will require the continued use, and eventual expansion of, the power reactor fleet to cover a significant portion of the baseload electricity demands. On the other hand, research reactors have been instrumental to scientific breakthroughs across almost all disciplines, are imperative for medical isotope production and essential testing grounds for future reactor and fuel designs.

Currently most power reactors run low enriched (LEU) UO_2 fuel pellets and the majority of research reactors use low-density, high enriched (HEU) uranium-silicide fuels. However, both these fuel concept have critical flaws and the communities are involved in dramatic fuel redesign processes. In the former case the Fukushima disaster prompted a significant drive to identify "accident tolerant fuels" with significantly improved thermal conductivity over UO_2. Research reactors, however, present high neutron flux requirements which currently necessitates the use of high uranium enrichment levels thus posing a significant proliferation risk. Here the challenge is to identify fuels with sufficiently improved uranium density to allow the transition to low enriched fuels, <20% U-235.

The leading candidates for research reactors are high-density, LEU U_3Si_2 or metallic U-Mo alloy concepts [1,2], whereas LEU U_3Si_2 and UN concepts have been identified as the most promising candidates for power reactor conversion [3]. Our understanding of these materials at a microscopic level is rapidly improving. However, only limited experimental effort has been expended to explore the structure of these materials at an atomic level, probe deviations from the global crystal structure, and understand fundamental properties such as their lattice dynamics. To this end, we have investigated two of the key fuel candidates, U-Mo and U_3Si_2 utilising the unique capabilities of the ID28 beamline. We have uncovered extensive local correlations through diffuse scattering studies, mapped out the previously unreported phonon dispersions via inelastic scattering experiments and coupling this with state-of-the-art *ab initio* calculations demonstrated significant disorder-phonon coupling in both systems [4,5]. These insights into the basic properties of these complex material systems should be considered when developing fuel performance codes or assessing in-reactor behaviour.

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Probing the interplay of static disorder with lattice dynamics using inelastic X-ray and neutron scattering

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An accurate description of both static and dynamic disorder is required to accurately describe soft framework materials [1]. To predict their properties – thermal expansion, ferroelectricity, etc. – it is useful to accurately measure their structure over a large range of timescales [2,3]. By combining diffuse and inelastic scattering, one can experimentally distinguish between the static and dynamical contributions to disorder. We apply this approach to the framework materials $Cd(CN)_2$ and $NH_4Zn(HCOO)_3$, both of which have static and dynamic disorder. We use inelastic neutron and X-ray scattering to study each of these systems respectively, revealing signatures of the interplay between dynamical processes of very different timescales. Methods for managing radiation damage in inelastic X-ray scattering (IXS) experiments on soft materials are discussed. The experiments are compared with lattice dynamical simulations designed to model both fast (~fs) and slow (~ms) dynamical processes. The approach is applied to explain the large isotropic negative thermal expansion in $Cd(CN)_2$ [4] and ferroelectricity of $NH_4Zn(HCOO)_3$ [5].
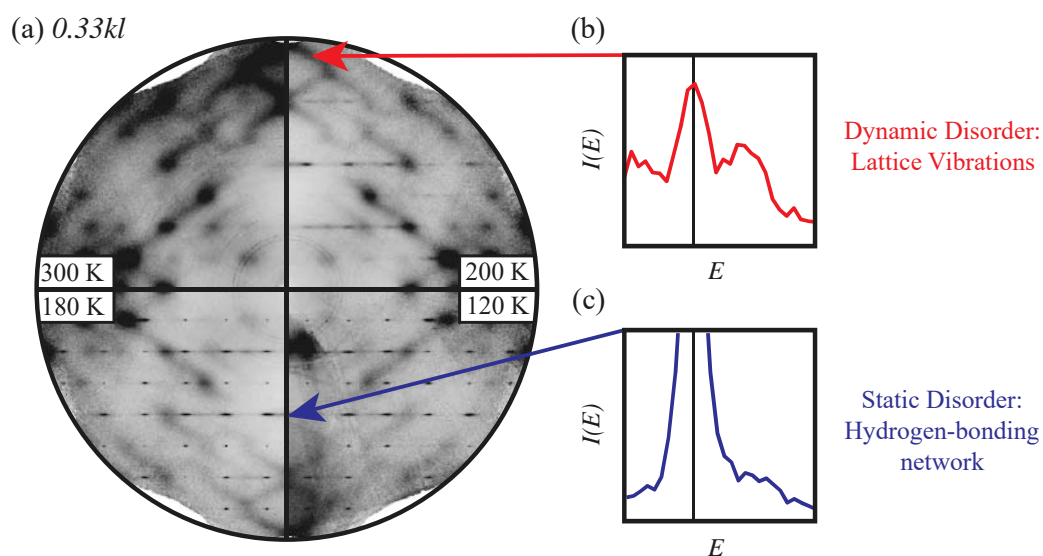
Figure 1: (a) A plane of diffuse scattering containing static and dynamic contributions to lattice dynamics: the broad diffuse scattering arises from the lattice dynamics and the sharp planes from static correlations of the hydrogen bonding network. (b-c) IXS can demonstrate this difference by measuring the energy dependence of each contribution, allowing for the distinction of the lattice vibrations from static disorder.

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Supercell lattice dynamical calculations to predict thermal diffuse scattering in materials with correlated disorder

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The analysis of diffuse scattering in compounds with substitutional disorder mainly focuses on the static description of local chemical environments, while the changes to the dynamics of the system due to correlated disorder are widely ignored. However, it is clear from supercell lattice dynamical calculations [1], that correlated disorder affects the phonon dispersion, as different degrees of band splitting and/or broadening are observed depending on the degree and nature of local order.

Using the solid solution series $KBr_{1-x}Cl_x$ ($0 \leq x \leq 1$) as a model system, we use supercell lattice dynamical canulations to demonstrate the effect of correlated short-range order on the first order thermal diffuse scattering [2]. We show that the correlated disorder significantly affects the dynamics in a system and cannot be modelled by the commonly used virtual crystal approximation. To furthermore demonstrate the viability of our model approach, we investigate the differences in the thermal diffuse scattering depending on different cation configurations in the mineral olivine $(Fe_{0.5}Mg_{0.5})_2SiO_4$ (see Figure 1).
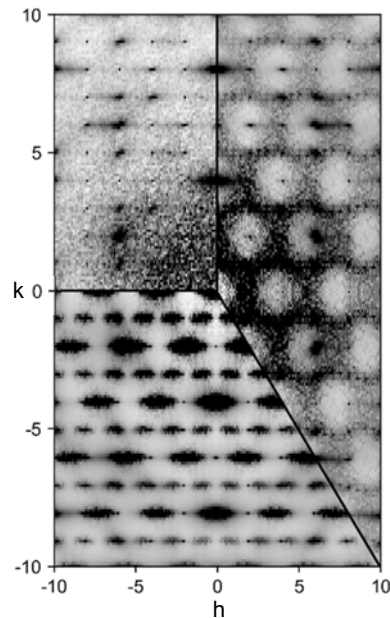
Figure 1: Predicted diffuse scattering in the *hk*0-layer of Olivine including contributions from static and dynamic disorder. Upper left: random distributed cations, upper right: high probability for different neighbouring cations, bottom left: high probability for identical neighbouring cations.

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Thermal diffuse scattering of framework materials: a coarse-grained approach

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Diffuse scattering contains information about static and dynamic correlations within a crystal. The dynamic contribution (thermal diffuse scattering, TDS) is dominated by low-energy vibrational modes. These modes are often key to the mechanical flexibility of solids, and so understanding their nature and microscopic origin is an important step in functional materials design.

This contribution will describe the development of an automated coarse-graining approach, which aims to capture the key low-energy dynamics of framework materials and allow validation of this interpretation in terms of the TDS component of single-crystal X-ray diffraction measurements. For framework materials, the low-energy modes tend to be associated with parallel motions of atoms at the nodes. This is true for inorganic solids ($Zn(CN)_2$, H_2O) [1,2], molecular systems [3] and metal–organic frameworks [4] alike. The proposed coarse-graining is straightforward: we keep the atoms at the nodes and replace the linkers with springs of fixed stiffness. Assigning a smaller energy penalty to framework hingeing, one can calculate the coarse-grained phonon dispersion of the framework structure, and thus the form of the thermal diffuse scattering. An example of the comparison between experiment and calculation is shown in the Figure. The method, that only requires a structure as an input, allows a straightforward approach for approximating TDS and for its interpretation in terms of whole-framework breathing and/or flexing modes. Its effectiveness will be discussed for a variety of chemically-different framework materials and whether this simple model can reproduce experimental results.
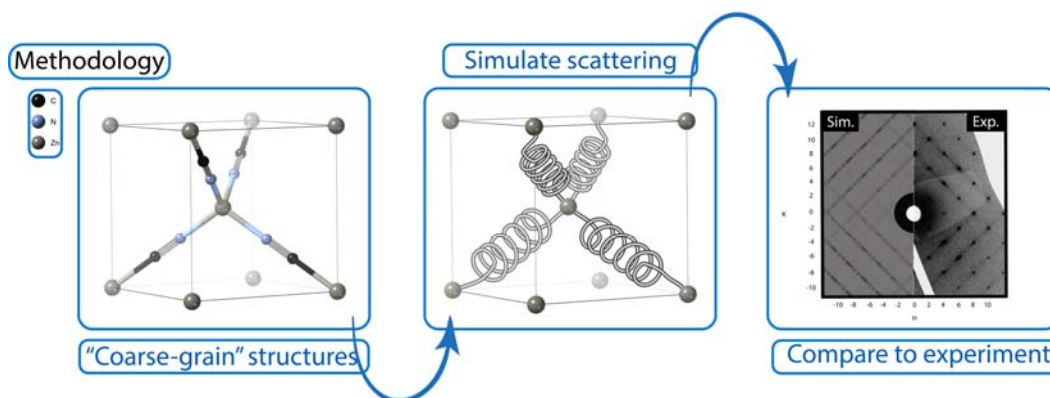
Figure 1: Overview of the methodology

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Phonon dispersion relations of novel phases in 1D nanosystems. Case study: wurtzite InP nanowires

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The recent upgrade of the ESRF source has paved the way to unprecedented scientific opportunities, only limited to the extent of our imagination. Inelastic x-ray scattering in grazing incidence was first applied at ESRF in 2005 to investigate the effect of the formation of charge density waves in the surface phonon dispersion relations of $NbSe_2$ [1]. Since then, only a handful experiments were realized worldwide to exploit the potential of this technique to investigate epitaxial films, such as InN [2], and uranium-based thin films [3]. The higher flux of ESRF-EBS allows now one to tackle the properties of systems in the nanoscale.

We report here the phonon dispersion relations of wurtzite-type InP nanowires (NWs) determined at beamline ID28 at ESRF by grazing incidence IXS with the aid of *ab initio* calculations and thermal diffuse scattering. To this aim, an nearly perfect 10x10 mm^2 array of wurtzite (wz) InP NWs on a zincblende InP substrate was grown using a gold seeded vapor-liquid-solid growth mechanism in a vapor-phase epitaxy reactor. This way, the NWs were aligned along the <111> direction and presented a super-crystal structure with properties similar to those of a hollow single crystal. The sample orientation and excellent crystalline quality was confirmed by thermal diffuse scattering (TDS). Despite a significant concentration of stacking faults and some spurious zincblende phase nano-segments in the nanowires, the outstanding quality and accurate crystallographic alignment of the NWs due to a precise control of the growth process allowed the determination of the acoustic phonon dispersion relations for the main symmetry directions, i.e. Γ-M, Γ-K-M, and Γ-A.

This pioneering experiment opens a pathway to ascertain the phonon dispersion relations of novel crystal phases, only accessible in one-dimensional systems.
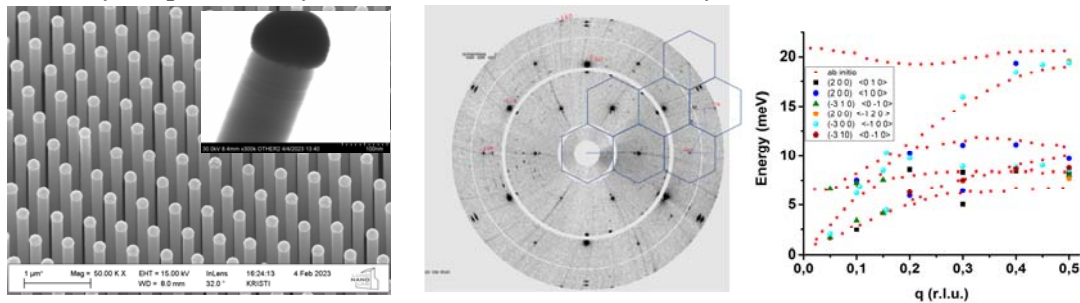
Figure 1: (left) Scanning electron microscopy images of the wz InP NW array grown on zincblende (zb) InP substrate. The inset shows a magnification of a single NW tip showing the gold seed and dark transverse lines revealing stacking faults with spurious zb phase sections. (center) TDS image displaying the main wz Bragg peaks in the HK0 plane. (right) Phonon dispersion relations of wz-InP NWs along the Γ-M direction (<100>).

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Evolution of charge order from underdoped to extremely overdoped region of the cuprate superconductor $La_{2-x}Ca_xCuO_4$

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The interplay between charge density wave (CDW) order and superconductivity in cuprates has been a subject of wide debate. Most early studies observed the disappearance of CDW just above optimal doping and well below the doping at which superconductivity disappears [1]. This brought into question the role of CDW in shaping the superconducting dome of the cuprates. Intriguingly, several recent studies in overdoped cuprates have found the existence of CDW in the overdoped regime [1-5], thus reviving the question of CDW as an order competing against superconductivity also on the overdoped side of the phase diagram. In this talk, I will report on our resonant x-ray scattering study of CDW in highly overdoped $La_{2-x}Ca_xCuO_4$ (LCCO) thin films, in which superconductivity remarkably persists to a doping of at least $x \sim 0.50$ with $T_c \sim 15$ K (Fig. 1) [6]. We find that CDW persists to a doping at least as high as $x = 0.50$, with distinct in-plane and out-of-plane correlations compared to bulk single crystals. The CDW intensity is strongly temperature dependent in the underdoped regime and becomes nearly temperature independent for $x = 0.30$ and above. Furthermore, the CDW wavevector is observed to lock into a commensurate $q \sim 0.25$ at high doping. I will discuss the general implications of these findings.
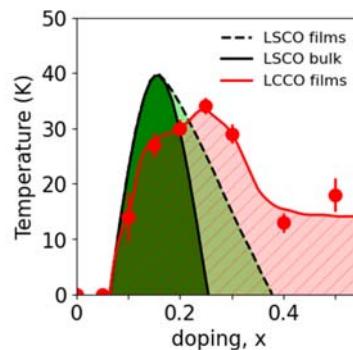
Figure 1: Doping dependence of superconducting T_c in LCCO, compared with that of bulk $La_{2-x}Sr_xCuO_4$ (LSCO) and LSCO films [6].

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Charge density waves and soft phonon evolution in the superconductor $BaNi_2(As_{1-x}P_x)_2$

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The superconductor $BaNi_2As_2$ (Tc = 0.6 K), an isostructural analogue to the parent compound of Fe-based superconductors $BaFe_2As_2$, exhibits an incommensurate charge density wave (I-CDW) and a commensurate CDW (C-CDW) accompanied with a transition to an orthorhombic and triclinic phase, respectively [1-2]. The CDWs and structural phases can be tuned by chemical substitution of e.g. arsenide with phosphorus. For phosphorus concentrations larger than ~7% the transition from the I-CDW to the C-CDW is suppressed while T_c jumps to ~3.2 K [3]. Recent investigations revealed that the I-CDW is associated with the softening of a low-lying optical phonon, which also displays an anomalously large splitting at the Γ-point [4-6]. However, DFT calculations indicate that the mechanism underlying the formation of the I-CDW is unconventional in nature [5].

We use diffuse and inelastic x-ray scattering to study the formation of the I-CDW and C-CDW in $BaNi_2(As_{1-x}P_x)_2$ for different substitution levels up to x≈0.1. We present the evolution of the diffuse scattering related to the I-CDW through the complete substitution series up to x≈0.1, evidencing a continuous lowering of the I-CDW transition temperature. Our inelastic x-ray scattering measurements at the transition from the I-CDW to the C-CDW show a sudden softening of the low-lying optical phonon branch at the C-CDW position without any indications of a softening at this wavevector above the transition temperature. Finally, we find a similar soft phonon driving the I-CDW in the absence of the transition to the C-CDW/triclinic phase (x≈0.1) down to 2.2 K.

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User-Dedicated Microsymposium UDM 4

7 February 2024

Introduction to the ESRF HOAHub: Creating an Atlas of Human Organs in Health, Ageing and Disease

UOC Organiser	Barbara Fayard
ESRF Organisers	Hector Dejea
	Paul Tafforeau
Non-ESRF Organisers	Joseph Brunet
	Peter Lee
	Xue Ruikang
	Claire Walsh
Venue	CIBB Meeting room

- Programme
- Abstracts of Keynote & User Talks

Introduction to the ESRF HOAHub:
Creating and Atlas of Human Organs in Health, Ageing and Disease

Wednesday, 7th February 2024 - Microsymposium UDM4
CIBB meeting room

Time	Session	Speaker
08:30 - 09:00	Registration and Welcome in CIBB meeting room	
09:00 – 09:10	Introduction to HOAHub & How to apply	Prof. P. Lee
09:10 – 09:20	Introduction to HiP-CT	Dr. C. Walsh
9:20 – 09:40	Keynote 1 (Brain)	Prof. A. Yendiki
09:40 – 10:00	Keynote 2 (Lung)	Prof. S. Verleden
10:00 – 10: 15	Coffee Break	
10:15 – 10:35	Keynote 3 (Image Processing)	Prof. J. Sporring
10:35 – 10:55	Round table discussion: Is your biomedical challenge appropriate for HiP-CT?	Keynotes & ESRF/ UCL staff
10:55 – 11:00	Mini-Coffee break	
11:00 – 11:45	Lab and BM18 tours	Dr. J. Brunet / Dr. H. Dejea
11:45 – 12:45	Hands-on HOA data download and visualization demo	Dr. J. Brunet / Dr. H. Dejea
12:45 – 13:00	Closing remarks	Prof. M. Ackermann

Large-scale imaging of neural circuits, from micro to macro

Anastasia Yendiki

Harvard Medical School, Mass General Hospital: **ayendiki@mgh.harvard.edu**

Hierarchical phase-contrast tomography (HiP-CT) has been introduced to scan entire human organs with near microscopic resolution. Initially, HiP-CT was specifically used to investigate the morphological changes in COVID-19 victims. Analysis of HiP-CT scans showed the existence of specific vascular and lobular changes within the lung. This proof-of-concept spurred interest in further analysis of neoplastic and non-neoplastic lung diseases. Indeed, HiP-CT can be leveraged to directly correlate radiologic changes to histopathology in 3 dimensions with high resolution. In addition, it also allows the investigation of the morphological changes in the airways, the vessels and the parenchyma. Within this talk we will focus on showing the initial experience of HiP-CT in COVID-19 lungs, but we will also highlight how HiP-CT can be used to study non-neoplastic lung diseases with case-studies of different chronic lung diseases.

Towards a better understanding of lung pathology applying
3- dimensional imaging

Stijn Verleden[1]

Antwerp Surgical Training, Anatomy and Research Centre (ASTARC) : **Stijn.Verleden@uantwerpen.be**

Hierarchical phase-contrast tomography (HiP-CT) has been introduced to scan entire human organs with near microscopic resolution. Initially, HiP-CT was specifically used to investigate the morphological changes in COVID-19 victims. Analysis of HiP-CT scans showed the existence of specific vascular and lobular changes within the lung. This proof-of-concept spurred interest in further analysis of neoplastic and non-neoplastic lung diseases. Indeed, HiP-CT can be leveraged to directly correlate radiologic changes to histopathology in 3 dimensions with high resolution. In addition, it also allows the investigation of the morphological changes in the airways, the vessels and the parenchyma. Within this talk we will focus on showing the initial experience of HiP-CT in COVID-19 lungs, but we will also highlight how HiP-CT can be used to study non-neoplastic lung diseases with case-studies of different chronic lung diseases.

On statistical summaries of collections of shapes in 3-dimensional images

Jon Sporring[1]

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With great advances in artificial intelligence, the field of image analysis is undergoing a rapid transformation, and segmentation models such as the UNet and Transformer models allow us to lift the gaze from voxels to the statistics, geometry, and topology of objects. In quantitative analyses of 3-dimensional image data, counting, shape measures, and their histograms are common in biological and material sciences, however, in most cases, the relation between objects cannot be ignored. The theory of spatial point processes offers a theory for point-like objects, such as objects of spherical shape of similar radii, where the second-order moment is often estimated using Ripley's K-function [Ripley 1976]. This function is useful for analyzing the tendency for points to cluster or repel each other at multiple scales and has been successfully applied in many domains such as [Khanmohammadi 2015, 2017]. However, it is difficult to apply to objects, which vary in shape and size. For images with many objects of general shapes, we review the Shape relation measure [Stephensen 2021], which is based on the intersection between r-parallel sets or dilations of a reference and observed objects and which we consider an extension of Ripley's K-functions to objects. A collection of r-parallel sets is a type of filtration in Topological data analysis [Edelsbrunner 2002] which together with the persistent homology barcode data structure is a promising tool for mixing geometry and topology for data analysis. As an example, we will end this talk by discussing recent work on a statistical summary of tube-like structures of potentially few but large objects [Wang 2024].

List of participants

Tutorials, Plenary Session
& User-Dedicated Microsymposia

List of Participants

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43	Maria Chrysina, Serena DeBeer	High-Energy Resolution Fluorescence Detected X-ray Absorption Spectroscopic Studies on Photosystem II
44	Abraham Nieva de la Hidalga, Leandro Liborio, Patrick Austin, Alejandra Gonzalez Beltran	Processing and analysis workflows that support reproducibility and replicability of published XAS results
45	Lindsay McGregor, Samira Acajjaoui, Ambroise Desfosses, Mélissa Saidi, Maria Bacia-Verloop, Jennifer J. Schwarz, Pauline Juyoux, Jill von Velsen, Matthew Bowler, Andrew A. McCarthy, Eaazhisai Kandiah, Irina Gutsche, Montserrat Soler-Lopez	Disassembling a complex I assembly factor: investigating the root causes of neurodegeneration
46	Rita Mendes Da Silva, Boram Yu, Mangalika Sinha, Daniel Fiole, Manfred Burgahmmer and Sarah Koester	Imaging biological cells using a custom-built beamline compatible microscope
47	Julien Orlans, Shibom Basu, Samuel Rose, Peter van der Linden, Daniele de Sanctis	Time-resolved tape-drive experiment at ID29 EBS-ESRF
48	Rive-Mathieu E, Jacquet P, Petit L, Engilberge S, Borel F, Cobessi D, Royant A	BM07-FIP2: A renewed versatile and tunable X-ray crystallography beamline at the ESRF
49	S. Engilberge, S.L. Rose, T. Giraud, P. Jacquet, N. Caramello, P. Carpentier, C. Mueller-Dieckmann, A. Royant	The icOS lab: A toolbox for (time-resolved) optical spectroscopy studies of proteins in crystallo
50	Jack Stubbs, Theo Hornsey, Niall Hanrahan, Luis Blay Esteban, Rachel Bolton, Martin Malý, Shibom Basu, Julien Orlans, Daniele de Sanctis, Jung-uk Shim, Patrick D. Shaw Stewart, Allen M. Orville, Ivo Tews, Jonathan West	Droplet microfluidics for time-resolved serial crystallography

Poster Number	Authors	Poster Title
51	Jack Stubbs, Martin Maly, Shibom Basu, Julien Orlans, Daniele de Sanctis, Ivo Tews	A user's perspective of SSX beamtime at ID29
52	Rachel Bolton, Jack Stubbs, Moritz Machelett, Danny Axford, Antoine Royant, Tobias E. Schrader, Takehiko Tosha, Hiroshi Suigimoto, Jonathan Worrall, Gwyndaf Evans, Michael Hough, Robin L. Owen, Ivo Tews	Making an enemy a friend: using photoreduction to reveal the Fe(II) and Fe(III) binding states of the FutA protein in marine cyanobacteria
53	Abigail SL Sudol, John Butler, Dylan P Ivory, Ivo Tews, Max Crispin	Extensive substrate recognition by the streptococcal antibody–degrading enzymes IdeS and EndoS
54	Matthew Rodrigues, Nitai Giri, Antoine Royant, Yang Zhang, Rachel Bolton, Gwyndaf Evans, Steve Ealick, Tadhg Begley and Ivo Tews	Trapping a novel intermediate of vitamin B6 biosynthesis in PLP synthase, using in crystallo spectroscopy
55	Hao Chen, Alessandro Chiasera, Francesco D'Acapito, Silvia Maria Pietralunga	Local structure of amorphous-to-crystalline WO3-x thin films studied by XANES and EXAFS
56	Maria C. Curria, Alejandro Fernandez-Martinez & Claire E. White	Elucidating hydrogenated structures: a multi-probe approach
57	Emmanuela Di Giorgio, Alberto Martinelli, Emanuela Sartori, Marta Campolucci, Maurizio Ferretti, Zeger Hens, and Federico Locardi	Structure Dynamics and Vibronic Coupling in AECuSi4O10 (AE: Ca, Sr, Ba) Compounds
58	L. Essaoui, J. Niyonzima, C. Tosarelli, C. Abadie, H. Jeridi, A. Vlad, A. Coati, Y. Prado, S. Royer, D. Constantin, I. Vickridge, M. Goldmann, Y. Garreau, D. Babonneau, B. Croset, E. Lhuilier, E. Lacaze	Organization of nanorods assemblies in liquid crystal topological defects
59	Olga Filimonova, Elena Bazarkina, Ruben Piña Garcia, Mauro Rovezzi, Valentina Batanova, Didier Wermeille	How Pt and As are hosted in pyrite, inclusions or solid solution?
60	Carolin Fischer, Maryam Tadayon, Luca Bertinetti, Yael Politi	Structure of cuticular mechanosensors in the spider Cupiennius salei
61	Moritz PK Frewein, Marc Allain, Asma A Medjahed, Britta Maier, Helmut Cölfen, Manfred Burghammer, Jeremy K Mason, Tilman A	Texture tomography for polycrystalline materials: Principle and first results
62	O. Irrazabal, O. Magnussen, C. Paetz, A. Sartori, J. Drnec	Operando XRD studies of catalytic dehydrogenation in LOHC technology
63	Inga Kicior, Veijo Honkimäki, Ardian Morina, Elizabeth Willneff, Peter J. Dowding, Sven L.M. Schroeder	Organic Friction Modifiers fundamentals studied by synchrotron X-ray scattering techniques
64	Zhao Li	Real-time Monitoring of Chemical and Local Structural Evolution during the Synthesis of Layered Li–Mn–Co–Ni oxides
65	Edouardos Loukopoulos, Sergio Marugán-Benito, Stefano Checcia, Ana E. Platero-Prats	Enhanced Capture of Persistent Water Contaminants Through Pore Environment Tuning of a Zr Metal-Organic Framework
67	C. Corley-Wiciak, M. H. Zoellner, A. A. Corley-Wiciak, E. Zatterin, I. Zaitsev, C. L. Manganelli, F. Rovaris, G. Nicotra, A. Marzegalli, D. Buca, F. Montalenti, T. U. Schulli, G. Capellini, and C. Richter	Case Study: Strain Tensor Mapping by Scanning X-ray Diffraction Microscopy on Group IV Micro-disks
68	V. Gonzalez, M. Cotte, F. Vanmeert, L. Monico6, C. Dejoie, M. Burghammer, W. de Nolf, L. Huder	The Heritage "BAG" at the European Synchrotron Radiation Facility: a new collaborative access modality for the structural analysis of historical materials
69	M. Cotte, H. Castillo-Michel, M. Salomé, G. Goulet, C. Holé, I. Fazlic, M. Wazne	The ID21 beamline: nano-spectroscopy with tender X-rays
70	Julio Cesar da Silva, Anico Kulow, Redhouane Boudjehem, Federico Monaco, Dmitry Karpov, Peter Cloetens, Jean-Louis Hazemann	Giga-voxel 3D imaging of samples larger and thicker than 100 microns by high-energy near-field Ptychographic X-ray Computed Tomography
71	Marina Eckermann, Takeshi Uenaka, Peter Cloetens, Marius Wernig	Multi-Modal characterization of brain organoids at the ESRF
72	Dmitry Karpov*, Marina Eckermann*, Deepak Mani, Rodion Shishkov, Sylvain Bohic, Alexandra Pacureanu, Lionel Andre, Murielle Salome, & Peter Cloetens	X-ray nano-imaging at ID16A: status and plans
73	Michael Grimes, Corentin Chatelier, Clément Atlan, Ewen Bellec, David Simmone, Kyle Olson, Steven J. Leake, Joël Eymery, and Marie-Ingrid Richard	Capturing catalyst strain dynamics during operando CO oxidation
74	Federico Castelli, Madeleine Han, Olga Stamati, Julie Villanova, Youssef Lahbib	Elemental distribution in seashells through nano-XRF and tomography
75	Dmitry Karpov, Ewen Bellec, Abisheik J. Samuel, Steven Leake, Peter Cloetens, Assaf Gal, Igor Zlotnikov	Role of lattice defects and chemical heterogeneity in asymmetric growth of biogenic crystals
76	Tang Li, Maik Kahnt, Thomas L. Sheppard, Runqing Yang, Ken Vidar Falch, Roman Zvagelsky, Pablo Villanueva-Perez, Martin Wegener, and Mikhail Lyubomirskiy	Challenges of X-ray multibeam ptychography at 20 keV

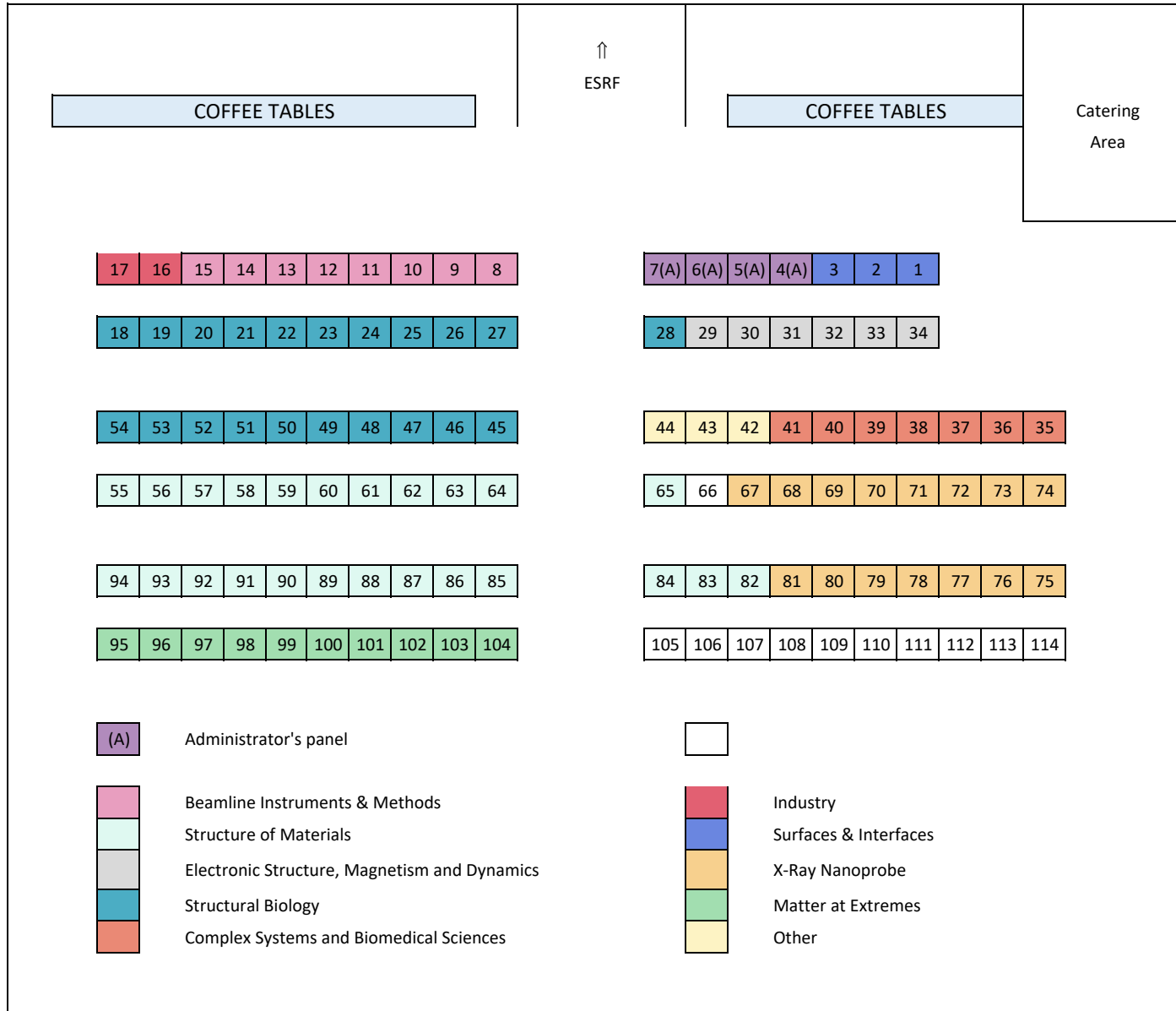| Poster Number	Authors	Poster Title
77	<u>M.-I. Richard</u>, C. Atlan, C. Chatelier, M. Grimes, E. Bellec, K. Olson, S. Yehya, D. Simonne, N. Vostrov, S. Labat, J. Carnis, L. Gao, M. Dupraz, L. Ni, S.J. Leake, E. Rabkin, O. Thomas, J. Eymery, T.U. Schülli	Structural Evolution of Nanoparticles Under Realistic Conditions Observed with Bragg Coherent X-ray Imaging
78	<u>Rodion SHISHKOV</u>, Dmitry KARPOV, Peter CLOETENS, Sylvain BOHIC	Deeply automated nanoscale X-ray fluorescence microscopy: from a few cells to statistical significance
79	<u>M. Stammer</u>, M. Frewein, I. Silva Baretto, S. Roffino, N. Wittig, C. Pedersen, H. Birkedal, M. Pithioux, T. Grünewald	The nanoscale architecture of the enthesis, the bone-tendon interface, probed with high resolution x-ray imaging
80	Edoardo Zatterin	Imaging strain with scanning diffraction microscopy
81	<u>Jiangtao Zhao</u>, Even Bellec, Marie-Ingrid Richard, Steven Leake and Tobias Schulli	Bragg Coherent Modulation Imaging for highly strained nanocrystals
82	<u>Sergio Marugán Benito</u>, Edouardos Loukopoulos, Ana Platero-Prats	Adsorption of emerging water contaminants using functionalized metal-organic frameworks via posrt-synthetic metalation
83	Marta Mirolo	ReMade@ARI: a hub for materials research dedicated to Circular Economy
84	<u>Marta Mirolo</u>, Alisson Iles Velez, Sergio F. Mayer	Analysis of the structural modifications of Na3PS4-based solid electrolyte during heating
85	<u>Annabel Olgo</u>, Quentin Jacquet, Quentin Berrod, Rasmus Palm, Sylvie Genies, Cédric Septet, Romain Franchi, Samuel Tardif, Claire Villevielle, Olivier Raccurt, and Sandrine Lyonnard	The Local Impact of Sensors on a Commercial Li-ion Battery Pouch Cell Graphite Electrode Lithiation Mechanism
86	<u>F. Pignon</u>, E. Guilbert, S. Mandin, F. Bosson, N. Hengl, M. Karrouch, B. Jean, J.L. Putaux, T. Gibaud, S. Manneville, T. Narayanan	Orthotropic organization of a cellulose nanocrystal suspension realized via the combined action of frontal ultrafiltration and ultrasound as revealed by in situ SAXS,
87	A. Rack	Beamline ID19: a versatile station for synchrotron-based full-field hard X-ray microimaging
88	<u>Raquel Rodriguez-Lamas</u>, David Bugallo, Eric Langenberg, Can Yildirim, Francisco Rivadulla, Carsten Detlefs	4D mapping of epitaxial stress relaxation through dislocation arrays in complex oxide superlattices
89	<u>P. Salles</u>, O. Irrazabal, M. Ronovski, I. Kicior, V. Manojlovik, F Rusello, A Sartori, V Vinci, M Mirolo, H Isern, V Honkimaki, J Drnec	ID31 - High-energy beamline for buried interface structure and materials processing
90	<u>Andrea Sartori</u>, Jakub Drnec, Joel Hatinen, Federica Mantegazzini	High energy X-ray characterization of interfaces in complex materials for quantum applications
91	<u>Oliver Spaeker</u>, Gavin J. Taylor, Bodo D. Wilts, Tomas Slaby, Mohamed Ashraf Khalil Abdel-Rahman, Ernesto Scoppola, Clemens N. Z. Schmitt, Michael Sztucki, Jiliang Liu, Luca Bertinetti, Wolfgang Wagermaier, Peter Fratzl, and Yael Politi	Structure-property-function relationships in the cornea of Limulus polyphemus
92	<u>J. Stickland</u>, D. Younas, Y. Chushkin, I. U. Hageberg, F. Zontone, S. Ucar, D. W. Breiby, B. Chattopadhyay	Nanoscale imaging of CaCO3 precipitation in the presence of Polystyrene Sulfonate
93	<u>A. Urbina</u>, S. Lorca, J. Abad, F. Santos, P. Almodóvar, C. Díaz-Guerra I. Galarreta, L. Cervera, J.Rubio-Zuazo and A.J. Fernández Romero	In operando XRD study of hexagonal MoO3-based and Bi2O3-based electrodes during Charge/Discharge processes of Zn batteries
94	<u>Valentin VINCI</u>, Marta MIROLO, Isaac MARTENS, Jakub DRNEC	High-energy scattering techniques to probe batteries, from capillary-sized cells to full packs
95	<u>L. Canet</u>, A.D. Rosa, G. Garbarino, A. Pokhamova, M. Gerin, M. Mezouar, G. Morard	Volatiles behavior during terrestrial evolution
96	<u>Xiang Li</u>, Ilya Kupenko	Complex electronic, magnetic, and structural transitions in FeO
97	<u>Emin Mijiti</u>, Fabienne Duc, Bastien Galaup, Olivier Mathon, Rafaella Torchio, Cornelius Strohm	XAS investigations of field induced valence transition in YbInCu4 under pressure
98	<u>Emin Mijiti</u>, Murat Durandurdu, Joao Elias F. S. Rodrigues, Angela Trapananti, S. Javad Rezvani, Angelika Dorothea Rosa, Olivier Mathon, Tetsuo Irifune, and Andrea Di Cicco	Structural and electronic changes in GeSe2 glass under ultra-high pressures probed by double-edge EXAFS measurements
99	<u>Susanne Müller</u>, E. Kolesnikov, X. Li, G. Aprilis, A. Chumakov, M. Mezouar, I. Sergeev, L. Libon, W. Morgenroth, A. Rohrbach, J. Berndt, M. Wilke, C. Sanchez-Valle, I. Kupenko	Sound velocities of iron alloys: Nuclear Inelastic Scattering at extreme conditions
100	<u>A.Pakhomova</u>, B.Journaux, T.Boffa Ballaran, I.E.Collings, S.Petitgirard, A.Kurnosov	Mineralogy of large icy satellites: insight from in situ X-Ray diffraction
101	<u>A.D. Rosa</u>, C.Clavel, A. Moyen, S. Pasternak, D. Buganez, F. Perrin, N. Sevelin-Radique, G. Morard, G. Garbarino, K. Lomachenko, O. Mathon	New opportunities for high pressure XAS at the ESRF-EBS and BM23 and ID24-DCM.

| Poster Number	Authors	Poster Title
102	S. Kamel, G. Caligari, L. Canet, S. Boccato, J. E. F. Rodrigues, E, Mijiti, M. Gerin, G.Garbarino, O. Mathon, M. Mezouar, A. D. Rosa, Guillaume Morard	Phase and spin transition in FeO at high pressure eludicated from XRD, XANES and EXAFS
103	Molokova Anastasia, Salusso Davide, Mathon Olivier and Lomachenko A. Kirill	In-situ and operando chemistry at BM23/ID24 XAS beamlines
104	R. Torchio, N. Sévelin Radiguet, J.A. Hernandez, S. Balugani, M. Masto, D. Bugnazet, S. Pasternak, F. Perrin, S. Chazalette, H. Gonzalez, E. Burtin, D. Lorphevre, C. Clavel, F. Villar, G. Berruyer and O. Mathon	The High Power Laser Facility at the ESRF

User Meeting 2024
Room Plan for Posters

⇑
ESRF

| COFFEE TABLES | | COFFEE TABLES | Catering Area |

| 17 | 16 | 15 | 14 | 13 | 12 | 11 | 10 | 9 | 8 |

| 7(A) | 6(A) | 5(A) | 4(A) | 3 | 2 | 1 |

| 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 |

| 28 | 29 | 30 | 31 | 32 | 33 | 34 |

| 54 | 53 | 52 | 51 | 50 | 49 | 48 | 47 | 46 | 45 |

| 44 | 43 | 42 | 41 | 40 | 39 | 38 | 37 | 36 | 35 |

| 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 |

| 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 |

| 94 | 93 | 92 | 91 | 90 | 89 | 88 | 87 | 86 | 85 |

| 84 | 83 | 82 | 81 | 80 | 79 | 78 | 77 | 76 | 75 |

| 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 |

| 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 |

Legend:

(A) Administrator's panel

Beamline Instruments & Methods

Structure of Materials

Electronic Structure, Magnetism and Dynamics

Structural Biology

Complex Systems and Biomedical Sciences

Industry

Surfaces & Interfaces

X-Ray Nanoprobe

Matter at Extremes

Other

Maps of Venues

- EPN Campus
- Tutorial Venues
- Plenary Session and UDM Venues

EUROPEAN PHOTON & NEUTRON SCIENCE CAMPUS - GRENOBLE
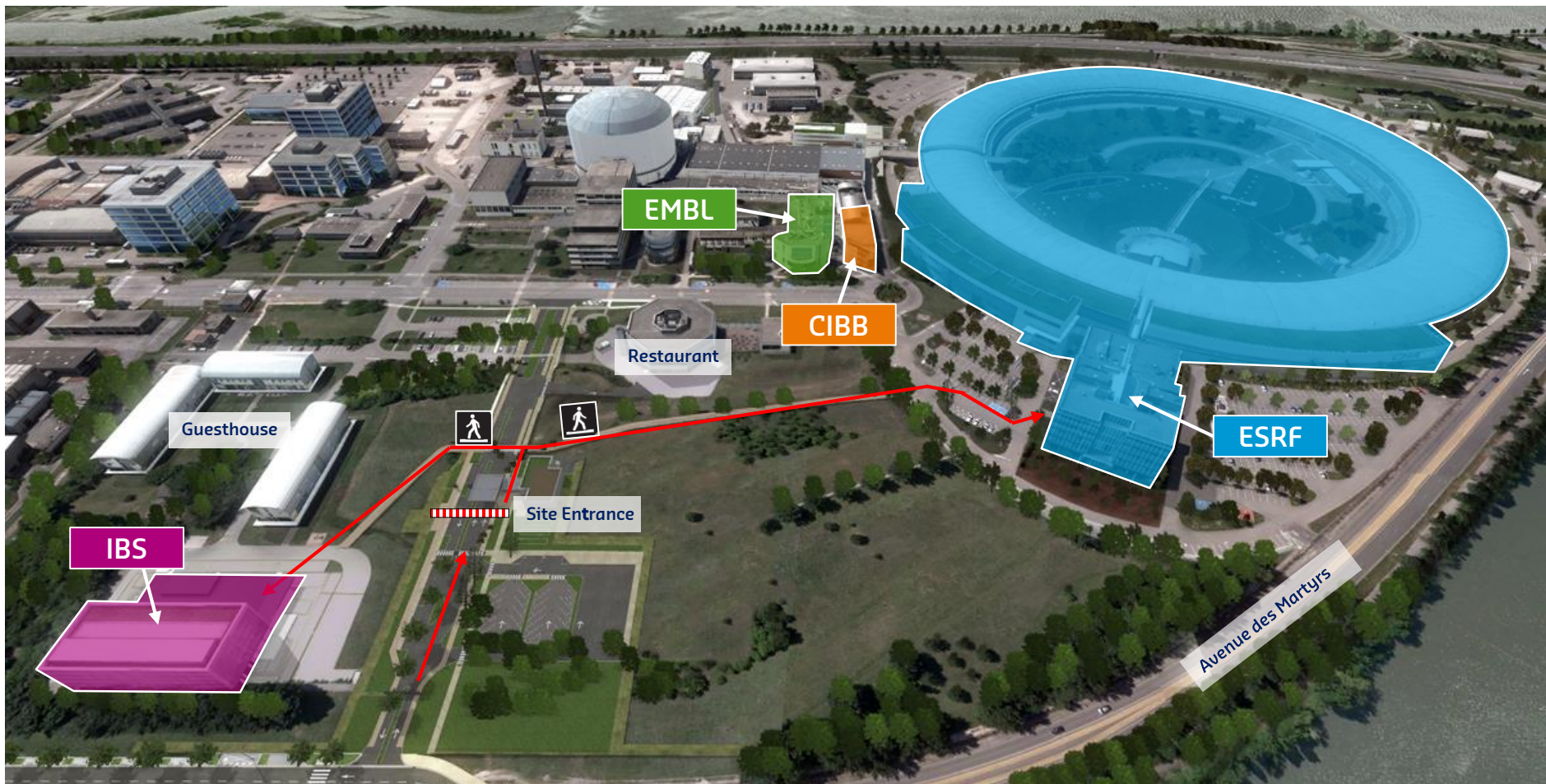
EMBL

CIBB

Restaurant

Guesthouse

Site Entrance

IBS

ESRF

Avenue des Martyrs

Grenoble downtown

Train station
Highway to Lyon
Shuttle from/to Lyon Airport
Shuttle from/to Geneva Airport
Tramway

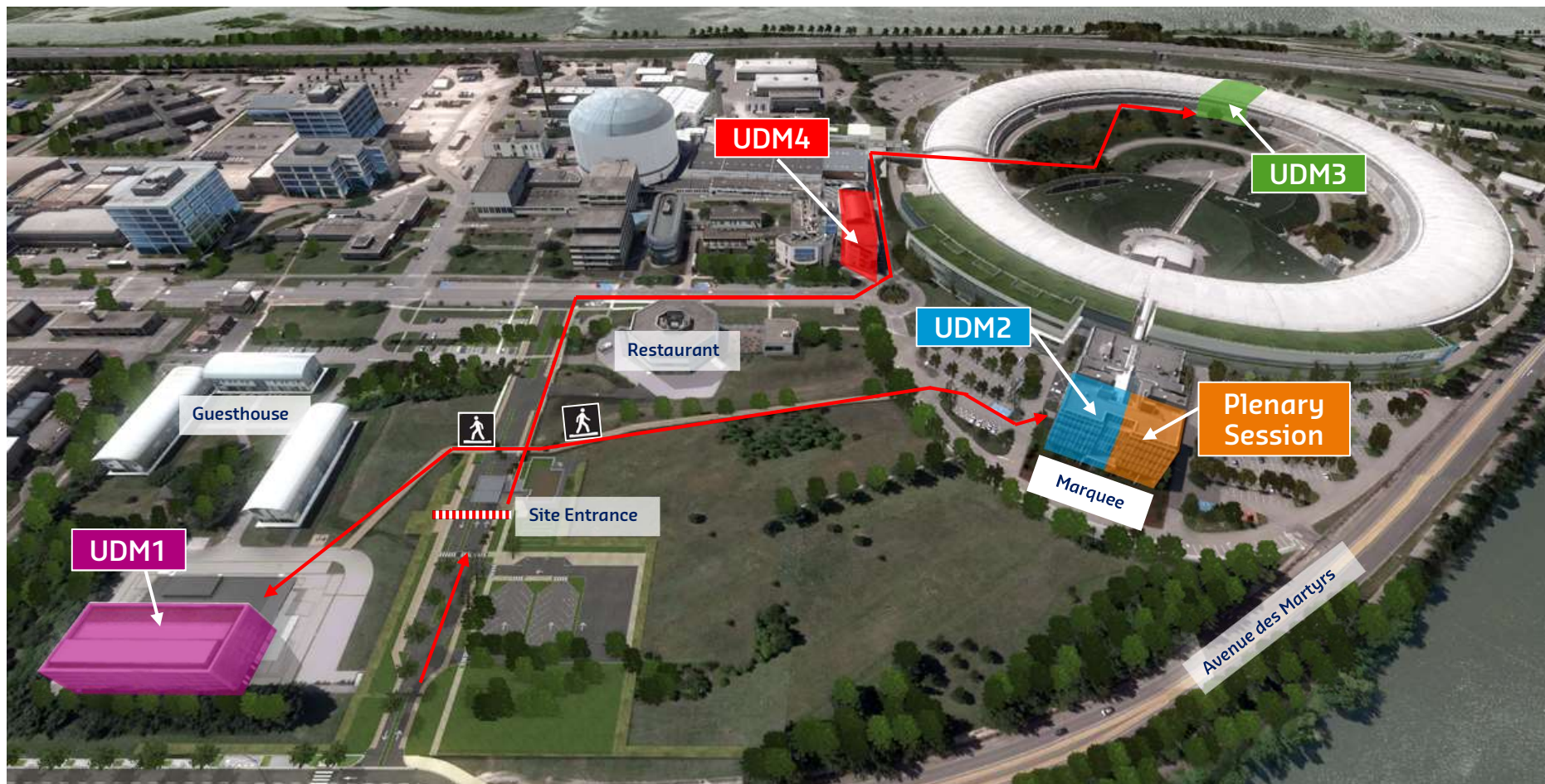**Highway**

To Chambery / Geneva

CIBB	Carl-Ivar Bränden Building – Partnership for Structural Biology
EMBL	European Molecular Biology Laboratory Grenoble
ESRF	European Synchrotron Radiation Facility
IBS	Institut de Biologie Structurale

USER MEETING 2024 – Tutorial Venues

T1	Volume image analysis of tomographic data	→ MD-1-21
T2	Structural Biology BAG meeting	→ CIBB Seminar room
T3A	Meet the Structural Biology scientists on the beamlines	→ Guided tour and Visitor Center
T3B	Demystifying the Structure-tO-Solution (SOS) pipeline	→ CIBB Seminar room
T4	How to write a news article about a scientific publication	→ LOB: Visitor Center
T5	Data reduction for scattering experiments using pyFAI	→ Central Building 3rd floor room 337
T6	XAS data analysis – common session	→ Central Building ESRF Auditorium
T7A	Introduction to the XAS technique and to the BM08/LISA beamline	→ Exp. Hall: BM08 Sec.07.5 room 7.5.02
T7B	Ab initio simulation of X-ray absorption spectroscopies using FDMNES	→ LOB: BEL-1-01
T8	XPCS: X-ray Photo Correlation Spectroscopy	→ EMBL Seminar room
T9	Nuclear resonance applications at the nanoscale inc. hands-on practical	→ Exp. Hall Sec.18 room18.1.11

USER MEETING 2024 – Plenary Session & Microsymposia Venues

UDM4

UDM3

UDM2

Restaurant

Guesthouse

Plenary Session

Marquee

Site Entrance

UDM1

Avenue des Martyrs

Grenoble downtown

Train station
Highway to Lyon
Shuttle from/to Lyon Airport
Shuttle from/to Geneva Airport
Tramway

Highway

To Chambery / Geneva

Plenary Session ⟶ ESRF Auditorium

UDM1 Towards filming macromolecular movies at the ESRF-EBS ⟶ IBS Seminar Room

UDM2 Machine learning and databases in X-ray spectroscopy ⟶ ESRF Auditorium

UDM3 The complementary use of diffuse and inelastic x-ray scattering ⟶ ESRF MD-1-21

UDM4 Introduction to the ESRF HOAHub: creating an Atlas of Human Organs in Health, Ageing and Disease ⟶ CIBB Meeting room