

ECA IET SIG No: 6

Reported Period: 08/2022 - now

Report Date: September 11th 2023

Reported by: Dr. Dubravka Sisak Jung, IET Sig 6 Secretary on behalf of the Sig 6 Members and the Sig 6 Chair Prof. Dr. Michele Cianci

1. Introduction.

ECA IET Sig6 Chair *Ullrich Pietsch* left its role and he was superseded by Prof. Michele Cianci.

ECA IET Sig6 Secretary *Michele Cianci* left its role and he was superseded by Dr. **Dubravka Sisak Jung**.

For 08/2022 - now *Michele Cianci's* and **Dubravka Sisak Jung's** work has included submission of the suggestions from the SIG to the Programme Chair of ECM34 Padova (Italy), one workshop and one school.

The Chair organized one crystallography school in Trieste for the Italian Crystallographic Association. Details below.

The Secretary chaired one workshop ("A practical approach to synchrotron experiments") at IUCR26 (Melbourne). Details below.

The Secretary is also member of the organizing committee of the Erice International School of Crystallography 2024. Details below.

2. SIG web site:

SIG 6's website is here:-

<https://ecanews.org/groups/sig-06-instrumentation-and-experimental-techniques/>

The 2018 to 2019 reports for example can be found here:

https://ecanews.org/wp-content/uploads/2019/08/Report-SIG6_2019.pdf

The report covering the 2020-21 period was submitted on the 8th of February 2021, but it has not been uploaded.

The reports covering the 2021-22 period was submitted on the 18th of July 2022, but it has not been uploaded.

3. Number of ECA individual members registered with the SIG

SIG 6 membership was 66 (checked on September 11th 2023).

4. Existence of a SIG mailing list?

Yes; the detailed instructions for using the email list can be found at the new ECA website and which are:-

Scientists which to participate to the SIG6 discussions should **join the group's mailing list**:

- mails can be sent to eca-sig6@listes.grenoble.cnrs.fr
- the archives can be consulted at <https://listes.grenoble.cnrs.fr/sympa/arc/eca-sig6> (subscribers only, and you need to create an account by clicking on the “first login ?” link at the top left)
- to **subscribe**, go to: <https://listes.grenoble.cnrs.fr/sympa/subscribe/eca-sig6>
- to **unsubscribe**, go to: <https://listes.grenoble.cnrs.fr/sympa/sigrequest/eca-sig6>

The mailing list engine is a SYMPA server, user information is available from: <https://listes.grenoble.cnrs.fr/sympa/help/user>

The list of commands you can send are listed in https://listes.grenoble.cnrs.fr/sympa/help/mail_commands (the list name is “era-sig6”)

6. List of MS proposed by the SIG for ECM34 Padova

Our Sig6 microsymbiosia proposals for the ECM34 Programme that we made in February 2023 are listed below:-

1. Artificial intelligence in photon and neutron crystallography (as per ECM 33).
2. The use of x-rays and neutrons for experiments in nanoscience (as in ECM32).
3. Crystallography at the nanoscale
4. Automation in data collection and processing
5. Time-resolved diffraction and scattering techniques
6. New detectors for X-ray and Electron applications.

7. Prizes awarded/sponsored/coordinated/received by Sig6 Members

At ECM33 Versailles the SIG6 poster prize, winner details and our judging panel are summarised below:-

SIG 6 Jacek Grochowski Poster Prize, 100 Euro

Judging Panel	Michele Cianci (Chair), Thompson Andrew, John Helliwell
Researcher	Dr. E. Wenger
MS and Poster	MS 40-1-4
Title	A unique laboratory experimental set up for single crystal diffraction under an electric field. Volta crystallography”

8. Past Activities other than Microsymposia at ECM

8.1 Schools

The details of AICS2022 International School of Crystallography organized by the Sig06 members are summarized as follow:

Title	Protein structure models, biophysical data and high-performance computing for drug design
Organisers:	Chair Dr. Paolo Mazzeo (University of Parma, Italy), Prof. Elisa Boanini, (University of Bologna, Italy), Prof. Michele Cianci (Università Politecnica delle Marche, Italy), Dr. Danilo Belviso (CNR – Bari).
Jointly with	none
When	Trieste (Italy) from the 7th of September till the 10th of September 2022
Partecipation fee	180 euro
Speakers	17
Attendees	30
Website	http://school2022.cristallografia.org/
Short description	The AICS2022 school focuses on the exploitation of protein structures, from crystallography, electron microscopy as well as biophysical data, molecular modeling and dynamics, for drug discovery; the aim of the school is to introduce young researchers from chemistry, structural biology, biophysics and biochemistry to the latest developments in the field, and provide a theoretical and practical overview of state-of-the-art tools in structure-based drug design, using both computational and experimental techniques.

The details of the Erice International School of Crystallography 2024 organized by the Sig06 members are summarized as follow:

Title	Powder Diffraction: Advancing Real Materials in the Information Era
Organisers:	Dubravka Sisak Jung (DECTRIS, Ltd), Prof. Dave Billing, (University of the Witwatersrand, South Africa), Prof. Matteo Leoni (Aramco, Italy)
Jointly with	none
When	Erice (Italy) from the 31 May - 8 June 2024

Partecipation fee	1250 Euro
Speakers	19
Attendees	n/a
Website	https://crystalerice.org/2024/
Short description	<p>Powder diffraction is one of the most flexible and widely employed tools for materials characterisation. Since its formal establishment over a century ago it has continuously evolved and contemporary applications include X-ray, neutron and electron diffraction and scattering modalities that find application in many research and industrial endeavours across a range of disciplines.</p> <p>Technical equipment and component advances coupled with developments in the fields of automation as well as information and data sciences have enabled experimental strategies that allow for measurements to be done in time or spatially resolved ways and which also incorporate control of external experimental parameters such as temperature, pressure, atmosphere or even magnetic or electrical fields. Readily producing a wealth of results amenable to analysis and interpretation via appropriate machine learning strategies and/or modelling of the structure/nanostructure aspects of even complex real materials of interest to industry and academia.</p> <p>This School aims to provide attendees with sound foundational understanding of the principles on which powder diffraction is based. It further seeks to showcase a selection of cutting-edge realisations of powder diffraction, including some newer hyphenated implementations that closely couple powder diffraction with complementary techniques such as tomography or various spectroscopies for an improved understanding of real material and the structural origins of their properties. Practically it seeks to provide the skills and knowledge needed to perform accurate measurements and using appropriate software and hardware tools, especially Rietveld and structure validation methodologies, to derive meaningful crystallographic results. And the school endeavours to gear attendees for future developments by formally including AI/ML and its use in the context of powder diffraction in the curriculum.</p> <p>The format of the School will include focussed lectures, expert panel discussions as well interactive hands-on sessions that will provide not only theoretical knowledge but also real practical opportunities to use some of the latest tools available to practitioners. Along with informal sessions intended to stimulate discussions between established experts, specialists, and the newer generations of researchers.</p>

8.2 Workshops

Title	“A practical approach to synchrotron experiments” at IUCR26 Melbourne
Organisers:	Dr. Dubravka Sisak Jung (DECTRIS) and Prof. Simon Grabowsky (Universität Bremen)
Jointly with	none
When	Monday, August 2, Time: 8:00am - 1:00pm
Participation fee	\$40AUD
Speakers	6
Attendees	60 registered participants
Website	https://iucr2023.org/workshops/
	https://swiss-crystallography.ch/en/uuid/i/ff5dfdc1-4017-5525-8ba7-ae24426a5b87-IUCr_workshop_%22Practical_approach_to_synchrotron_experiments%22
Short description	A wider availability of beamlines to users is enabled with more automated beamlines with remote access, mail-in services, multipurpose setups. Yet, the access to large-scale facilities remains competitive, many beamlines are overbooked, and each moment of a beamtime is precious. Moreover, the advent of 4th generation synchrotron sources brings other opportunities and challenges: (i) performing non-standard techniques (e.g. XRD/PDF-computed tomography, ptychography, in situ), (ii) shift of users during shutdowns and upgrades (iii) managing high-data volumes. In this context, meticulous experiment design and a high level of awareness are extremely important. Though many synchrotrons and beamlines have instructions on how to organize an experiment, this information can be too specific, or limited only to execution.

- Prof. John Helliwell completed four triennia leading IUCr discussions on raw diffraction data archiving, benefits and costs, as Chair of the IUCr Diffraction Data Deposition Working Group 2011 to 2017 and as Chairman of the IUCr Committee on Data 2017 to 2023.
- Prof. John Helliwell completed four triennia as IUCr’s Representative to the International Science Council’s Committee on Data, ‘CODATA’.
- Prof. John Helliwell completed ten years as Chairman of the European Spallation Source Scientific and Technical Advisory Panel for NMX (neutron macromolecular crystallography instrument).
- Prof. Naomi Chayen was a Member of the International advisory committee of The International Conference on Crystal Growth and Epitaxy-**ICCGE-20** in Naples in August 2023

10. Summary of Outreach activities

One Crystallographic School and workshop microsymbosia at IUCR26 were organized. Several other committees on crystallographic related matters were chaired.

11. Future/Programmed Activities.

A Sig 6 member, namely Michele Cianci is part of the organizing committee of ECM34 in Padova (IT). Sig6 is represented at the ECM34 Programme Committee by the newly appointed Sig 6 Chair.

12. Other contributions to crystallography

n/a

13. Other matters.

None to report.

14. Brief annual activity report

Our core function is to have assisted with the ECM next meeting program, ECM34.

We have been active in outreach.

Overall Sig6 shows a real willingness to integrate and collaborate with IUCr on the matters of policy re crystallographic data and which includes:- encouraging the availability of our raw diffraction data for all experimental methods of crystallography in addition to our processed diffraction data (such as structure factors or scattering curves/profiles) and our derived atomic and molecular data.

Michele Cianci, as member of the AIC Commission for Crystallography Teaching and the Scientific Committee of the School, is actively engaged in organizing the yearly schools of the Italian Crystallographic Association.

15. List SIG officers, name and e-mail, and specify their main function in the SIG:

Chair Prof. Dr. Michele Cianci m.cianci@univpm.it

Secretary Dr. Dubravka Sisak Jung dubravka.sisak@dectris.com

Immediate past Chair Prof. Dr. Dr. h.c. Ullrich Pietsch pietsch@physik.uni-siegen.de

Immediate past secretary Dr. Michele Cianci m.cianci@univpm.it

Members:-

Other members:

- Tilo Baumbach (D)
- Robert Cernik (UK)
- Naomi Chayen (UK)
- Vincent Favre-Nicolin (F) – webmaster
- Santiago Garcia Granda (SP)
- Heger Gernot (G)
- René Guinebretière (F)
- John R. Helliwell (UK)
- Jean-Louis Hodeau (F)
- Jordi Juanhuix (S)
- Martin Lutz (NL)
- Ake Kvik (S)
- Ian Robinson (UK)
- Juan Rodriguez-Carvajal (F)
- Emmanuel Saridakis (GR)
- Thomas Tschentscher (G)
- Heribert Wilhelm (UK)

Supplementary Materials.

None.