

ECA IET SIG No: 6

Reported Period: 08/2023 - now

Report Date: 5th August 2024

Reported by: Dr. Lucy Saunders, Diamond Light Source 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 remains Prof. Michele Cianci.
ECA IET Sig6 Secretary Dr. **Dubravka Sisak Jung**. left their role and were superseded by **Dr Lucy Saunders**

For 08/2023 - now **Michele Cianci's** and **Lucy Saunders's** work has included: 1) be part of the ECM-34 organizing committee (MC); 2) Coordination of Sig6 activities and representation of Sig6 at European meetings.

The Chair organized one crystallography school in Pisa, IT for the Italian Crystallographic Association. Details below.

The Secretary gave a lecture and was a poster judge at the Erice International School of Crystallography 2024 in Powder Diffraction.

2. SIG web site:

SIG 6's website is here:-

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

3. Number of ECA individual members registered with the SIG

SIG 6 membership includes **50 registered members** on the mailing list and **64 individual members** of ECA (from ecanews.org).

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 ECM35

Our Sig-06 microsytosia proposals for the ECM35 Programme are listed below:-

1. AI, software developments and Machine learning applied to MX and CryoEM (approved for per ECM 34).
2. AI and Automation in data collection and processing (approved for per ECM 34).
3. Future of light sources and XFEL (approved for per ECM 34).
4. In situ and Operando diffraction-(i.e. diffraction studies of working materials with simultaneous activity measurements. Not limited to powders). Time-resolved diffraction and scattering techniques. (approved for per ECM 34).

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

We reported the details of the winner at ECM33 in Versailles in the previous report. For ECM34 the SIG 6 Jacek Grochowski Poster Prize has been sponsored by CINEL Instruments, PD, ITALY. The Chair of the Poster Prize Committee will be Prof. John. R. Helliwell. Details of winner and our judging panel at ECM34 Padua the SIG6 poster prize, will be in the next report.

8. Past Activities other than Microsymposia at ECM

8.1 Schools

The details of AICS2023 International School of Crystallography organized by the Sig06 members are summarized as follow:

Title	ELECTRON CRYSTALLOGRAPHY A deep dive into nanocrystals
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	Pisa (Italy) from the 3rd of July till the 6th of July 2023
Partecipation fee	180 euro
Speakers	9
Attendees	15
Website	https://school2023.cristallografia.org/
Short description	<p>The AIC2023 School will focus on the currently available procedures for 3DED analysis.</p> <p>Students will be first introduced to the peculiarities of ED and then driven through data acquisition procedures and data reduction software. The school will cover both well-established 3DED protocols, based on step-wise acquisition and beam-precession, and more recent protocols based on continuous data acquisition through latest fast and sensitive detectors, particularly suitable for organics and macromolecules. Methods and routines for structure solution and refinement will be described, with a special focus on the treatment and use of residual dynamical effects. Specific features and issues related with inorganic, small-molecule organics and macromolecular compounds will be stressed. All these topics will be covered in frontal lectures and practical activities that will allow students to use first-hand several softwares for 3DED data reduction, structure solution and structure refinement. Students will also participate to lab activities, including 3DED data acquisition and advanced sample preparation for ED experiments. The last part of the school will finally introduce other cutting-edge methodologies, like serial-ED, phase-orientation mapping and electron pair-distribution function (ePDF).</p>

8.2 Workshops

- Prof. John Helliwell co-organized a workshop at the IUCr Congresss 2023 in Melbourne on Raw Diffraction Data Reuse

10. Summary of Outreach activities

One Crystallographic School was organized.

11. Future/Programmed Activities.

A Sig-06 member, namely Michele Cianci is part of the organizing committee of ECM34 in Padova (IT). Sig-06 is represented at the ECM34 Programme Committee by the newly appointed Sig-06 Chair.

12. Other contributions to crystallography

- Prof. John Helliwell acted in advisory committee roles as Chairman of the International Advisory Board of the Physical Sciences Data Infrastructure (PSDI) initiative and Member of the International Advisory Board for the DAPHNE4NFDI project in Germany.

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.

Lucy Saunders is the bursary secretary for the British Crystallographic Association (BCA) Council and an ordinary member of the BCA Chemical Crystallography Group committee, frequently involved in the chairing or organising of BCA annual and Autumn meetings.

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. Lucy Saunders lucy.saunders@diamond.ac.uk

Immediate past Chair Prof. Ulirch Pietsch Pietsch, pietsch@physik.uni-siegen.de

Immediate past secretary Dr. Dubravka Sisak Jung dubravka.sisak@dectris.com

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 Kvick (S)
- Ian Robinson (UK)
- Juan Rodriguez-Carvajal (F)
- Emmanuel Saridakis (GR)
- Thomas Tschentscher (G)
- Heribert Wilhelm (UK)

Supplementary Materials.

None.