

ECA IET SIG No: 6

Reported Period: 08/2024 - now

Report Date: 5<sup>th</sup> August 2025

Reported by: the Sig 6 Chair Prof. Dr. Michele Cianci on behalf of the Sig 6 Members

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## **1. Introduction.**

ECA IET Sig6 Chair remains Prof. **Michele Cianci**, Università Politecnica delle Marche (IT).

ECA IET Sig6 Secretary Dr. **Lucy Saunders**, Diamond Light Source (UK).

For 08/2024 - now **Michele Cianci's** work has included: 1) be part of the ECM-35 organizing committee (MC); 2) Coordination of Sig-06 activities and representation of Sig-06 at European meetings.

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

The Secretary is on maternity leave since the 5<sup>th</sup> August 2024.

## **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 **55 registered members** on the mailing list and **69 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](mailto: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](https://listes.grenoble.cnrs.fr/sympa/help/mail_commands) (the list name is “era-sig6”)

## 6. List of MS proposed by the SIG-06 for ECM35

Our Sig-06 microsymposia 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. List of MS approved by the organizing committee for ECM35

### **M3 Software developments in MX and Cryo-EM including AI / Machine Learning**

Chairs: Maria Fando (STFC-UKRI, Oxford, UK), Isabel Uson (IBMB-CSIC, Barcelona, ES);  
 Speakers: Lucrezia Catapano (MRC-LMB, Cambridge, UK), Sergei Grudinin (U Grenoble-Alpes, FR)  
 SIG-01,06

### **M36 In situ and operando diffraction; time- resolved techniques**

Chairs: Mattia Gaboardi (U Rome Tor Vergata, IT), Boby Joseph (Elettra, Trieste, IT) Speakers: Marco Giorgetti (U Bologna, IT), Umbertolucia Ranieri (MPC, Donostia- San Sebastian, ES)  
 SIG-06

### **M35 Challenges of light sources, neutrons and XFEL**

Chairs: Alke Meents (DESY, Hamburg, DE), + to be confirmed  
**SIG-01,06**

## **8. List of keynote speakers suggested by SIG-06 and approved for ECM35**

KL9 Toward understanding the Molecular Architecture of a glycogen- committed PP1/PTG holoenzyme: a Putative Target for Lafora Disease Paola Storici (Elettra, Trieste, IT), SIG-06

KL18 Bridging the gap. Serial crystallography at 4th generation synchrotrons: current status and future goals

Daniele de Sanctis (ESRF, Grenoble, FR), SIG-06

## **8. Prizes awarded/sponsored/coordinated/received by Sig-06 Members**

At the ECM-34 in Padua, the ET SIG 6 Poster Prize: Prof Jacek Grochowski In Memoriam prize was awarded to Dr. Eleanor Keil, The University of Southampton (UK) – Understanding Carbon Dioxide Uptake in ZIFs via In-Situ Single Crystal Diffraction. The judging panel was chaired by Prof. John Helliwell with dr. Adam Round (X-FEL, DESY, De) and dr. Lisa Vaccari (Elettra, IT). The prize consisted of a certificate and a lump sum of 150 euro after tax and was kindly supported by CINEL Strumenti Scientifici s.rl. Padova, Italy.

## **9. Past Activities other than Microsymposia at ECM**

### **9.1 Schools**

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

| Title                    | <b>International School on Current and Future Integrative Structural Biology (AICS2025)</b>                                                                                                                                                                                                                                                     |
|--------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Organisers:              | Chair Prof. Roberto Steiner (University of Padova, Italy), Prof. Michele Cianci (Università Politecnica delle Marche, Italy), Dr. Alessandro Grinzato (University of Padova, Ital.), Dr. Marco Mazzorana (Diamond Light Source, Didcot, UK), Sabrina Nazzareni (University of Parma, Italy), Aurelia Falcicchio (IC-CNR, Bari, Italy).          |
| When                     | Padova (Italy) from the 7th of July till the 11th of July 2025                                                                                                                                                                                                                                                                                  |
| Partecipation fee        | 490 euro                                                                                                                                                                                                                                                                                                                                        |
| Speakers                 | 14 (9 international, 5 Italian)                                                                                                                                                                                                                                                                                                                 |
| Attendees                | 32                                                                                                                                                                                                                                                                                                                                              |
| Website                  | <a href="https://school2025.cristallografia.org/">https://school2025.cristallografia.org/</a>                                                                                                                                                                                                                                                   |
| Supporting Organizations | Italian Crystallographic Association (AIC), International Union for Crystallography (IUCr), Elettra Synchrotron s.r.l. (Basovizza, Trieste, Italy), Società Italiana Biochimica (SIB)                                                                                                                                                           |
| Short description        | The 2025 edition placed a strong emphasis on <b>single-particle cryo-electron microscopy (cryo-EM)</b> , featuring dedicated lectures and hands-on computational practicals. Participants also benefited from sessions covering <b>X-ray and electron crystallography, X-ray tomography, cross-linking mass spectrometry</b> , and cutting-edge |

|  |                                                                                                                                                                                                                                                                                              |
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|  | applications of <b>machine learning and AI tools</b> in structural biology. The five-day program combined <b>morning lectures on theoretical fundamentals</b> with <b>afternoon tutorials and practical sessions</b> , offering an immersive experience in structural biology methodologies. |
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## 9.2 Workshops

None.

## 9.3. Summary of Outreach activities

One Crystallographic School was organized.

## 10. Future/Programmed Activities.

A Sig-06 member, Michele Cianci is part of the organizing committee of ECM36 in Prague (CZ). Sig-06 is represented at the ECM36 Programme Committee by the newly appointed Sig-06 Chair.

## 11. Other contributions to crystallography

- Prof. John Helliwell has continued representing IUCr at UNESCO's Open Science Workshops, with relevance to open access publication, open data, open software and open instrumentation (formerly the Global Commons).
- Prof. John Helliwell has two new books
  - *Certifying Central Facility Beamlines for Biological and Chemical Crystallography and Allied Methods*, IUCr Springer Briefs in Crystallography <https://link.springer.com/book/10.1007/978-3-031-80181-5>
  - *Precision and Accuracy in Biological Crystallography, Diffraction, Scattering, Microscopies, and Spectroscopies* IUCr Book Series Teaching Text, OUP <https://global.oup.com/academic/product/precision-and-accuracy-in-biological-crystallography-diffraction-scattering-microscopies-and-spectroscopies-9780198952824?lang=en&cc=gb#>
- Prof. Naomi Chayen recently developed new methods for crystallization for drug discovery: <https://www.imperial.ac.uk/news/265335/research-reveals-pneumonia-drug-fights-infection/>
- Prof. Michele Cianci is currently working as consultant for Elettra Synchrotron s.r.l. (Basovizza, Trieste, Italy) to develop uXRD beamline following the Elettra 2.0 upgrade.

## 12. Other matters.

None to report.

## 13. Brief annual activity report

Our core function is to have assisted with the ECM next meeting program, ECM35.

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.

**14. 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. Ulrich Pietsch* Pietsch, pietsch@physik.uni-siegen.de

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.