

# SIG4 activity report September 2023-September 2024

## Editorial activity of SIG members

**Xiaodong Zou:** main editor, section for Electron crystallography, IUCrJ

**Mauro Gemmi,** co-editor, section for Electron crystallography, IUCrJ

**Louisa Meshi,** co-editor, section for Electron crystallography, IUCrJ

**Lukas Palatinus:** co-editor of Acta Cryst A (IUCr)

**Tatiana Gorelik:** co-editor of Acta Cryst A (IUCr)

**Joke Hadermann:** co-editor of Acta Cryst B (IUCr), *J. Solid State Chem.* (Elsevier), *Batteries* (MDPI), *Springer Briefs in Crystallography*

**Hongyi Xu:** co-editor of Acta Cryst D (IUCr)

**Tatiana Latychevskaia,** editor of *Scientific Reports*

**Damien Jacob,** co-editor in chief of the *The European Physical Journal Applied Physics* (EPJAP)

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## Organization of ECM

SIG4 representative in the organizing committee of ECM34 in Padova 2022 – [Anton Cleverley](#)

List of MSs @ECM33 organized by SIG:

- M15 “*ED small waves, big ponds – Biomolecules and macromolecules*” Chairs: Dominique Housset (IBS, FR)
- M16 “*Method development and instrumentation in the world of electron diffraction*” Chairs: Mariana Klementova (FZU, CZ)
- M19 “*Advanced and new techniques to study inorganic and magnetic crystal structures*” Chairs: Gladys Steciuk (FZU, CZ), Enrico Mugnaioli (University, Pisa, IT), Françoise Damay (CEA, FR)
- M20 “*When can ED challenge XRD in small molecule crystallography?*” Chairs: Arianna Lanza (Copenhagen University, DK), Tim Gruene (University of Wien, AT)
- M21 “*Electron diffraction joining forces with quantum crystallography towards materials science applications*” Chairs: Richard Beanland (University of Warwick, UK), Paulina Dominiak (University of Warsaw, PL)

KeyNote Speaker: Louisa Meshi (University of the Negev, IL)

SIG4 representative in the organizing committee of ECM35 Poznan / Lviv 2025 – [Sergi Plana Ruiz](#)

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## SIG4 webpage and mail list

Webpage is on and frequently updated. Webpage administrator Tim Gruene.

<https://eaelectronsig.wordpress.com/>

Mail list administrator is Jérôme Pacaud [jerome.pacaud@univ-poitiers.fr](mailto:jerome.pacaud@univ-poitiers.fr)

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## Prizes sponsored/coordinated

SIG4 distinguished publication award 2024 will be announced at the ECM34, the chair of the price committee is Stéphanie Kodjikian.

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## Organization of dedicated schools / workshops

- 3D ED/MicroED workshop at the Australian Cryo-EM meeting (CryOZ), Australia, 23 Nov 2023

*Level of involvement of SIG in the activity:* SIG4 member in the organization and teaching (Hongyi Xu)

*ECA Individual Members registered with the SIG involved in the organizing committee:* yes

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed (SIG logo on the web page/leaflets):* no

*Sponsored by ECA (Yes/ No)?* no, not applied for

- Practical course “3D electron diffraction in Materials science” (Grenoble, France, 2 sessions (6-7/11/2023 & 4-6/06/2024), 4 participants per session)

*Number of participants:* 8

*Level of involvement of SIG in the activity:* 2 SIG4 members in the organization and teaching (Stéphanie Kodjikian and Christophe Lepoittevin)

*ECA Individual Members registered with the SIG involved in the organizing committee:* yes

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed (SIG logo on the web page/leaflets):* no

*Sponsored by ECA (Yes/ No)?* no, not applied for

*Short description:* Training workshop for X-rays crystallographers focused on the practical aspects of 3D electron diffraction in materials science, with alternation of demonstrations and manipulations on TEM, and tutorial sessions on computer.

*Web address:* <https://cdifx.univ-rennes1.fr/RECIPROCS/RECIPROCS.htm>

- 3D-ED Workshop ICIQ Tarragona, Spain, 23-26 October, 2023

*Level of involvement of SIG in the activity:* SIG4 members in the organization and teaching (Jordi Benet-Buchholz, ...)

*ECA Individual Members registered with the SIG involved in the organizing committee:* yes

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed (SIG logo on the web page/leaflets):* no

*Sponsored by ECA (Yes/ No)?* no, not applied for

*Short description:* We are thrilled to announce the first Workshop on Electron Diffraction for Structure Resolution taking place at ICIQ in Tarragona on October 23-26, 2023.

This workshop will focus on the practical aspects of electron diffraction along with some underlying theory. The workshop will be open to beginners and experts alike but a background in X-ray crystallography can enhance the learning experience.

Workshop discussions will encompass:

The roots of 3D-ED

Sample Measurement and Preparation

Types of samples suitable to be measured

Software applications

Kinematical and dynamical refinements

Understanding of absolute structure and configuration

Practical sessions on measurements and sample cryo-preparation

The event will feature insightful lectures from renowned professionals in electron diffraction. Attendees will also get the chance to familiarize themselves with an electron diffractometer, the Rigaku XtaLAB Synergy-ED.

For those interested in 3D-ED but lacking a crystallography background, hands-on sessions offer a gateway into the methodology and a firsthand experience with the Synergy-ED.

*Web address:* <https://www.iciq.org/agenda/3d-ed-workshop/>

- The 26th ECA Lunch webinar 15 February 2024, online, Sergi Plana Ruiz: "Liquid phase electron crystallography: the path to electron diffraction from protein crystals at room temperature"

*Number of participants:* 46 attended / 69.

*Web address:* [https://ecanews.org/education/eca-lunch-webinars\\_past-events/#26th-webinar](https://ecanews.org/education/eca-lunch-webinars_past-events/#26th-webinar)

- NordTEMhub/ARTEMI Workshop held on Three-Dimensional Electron Diffraction, Stockholm, 15-17 April, 2024

*Number of participants:* 45 participants from 10 different countries

*Level of involvement of SIG in the activity:* SIG4 members in the organization and teaching (Tom Willhammar, Hongyi Xu and Xiaodong Zou)

*ECA Individual Members registered with the SIG involved in the organizing committee:* yes

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed (SIG logo on the web page/leaflets):* no

*Sponsored by ECA (Yes/ No)?* no, not applied for

*Short description:* The workshop covers the fundamentals of crystallography, electron diffraction, and structural analysis by 3D ED. The workshop includes two afternoon practical sessions, from demonstrations of sample preparation and data collection in small groups (6-8 people/group), to hands-on computer sessions covering data analysis and structure determination. The last day included talks on the recent developments of ED-based methods and their applications on different materials.

*Web address:* <https://artemi.se/workshop-held-on-three-dimensional-electron-diffraction/>

- Workshop on Advanced Precession-Assisted 4D-STEM and 3D-ED, 19 - 20 June 2024, FZ Juelich, Germany (hybrid).

*Number of participants:* 60 (in-person), 120 registered on-line participants (come and go, simultaneous on-line participation was around 60).

*Level of involvement of SIG in the activity:* SIG4 members involved in the teaching

*ECA Individual Members registered with the SIG involved in the organizing committee:* no

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed (SIG logo on the web page/leaflets):* no

*Sponsored by ECA (Yes/ No)?* no, not applied for

*Short description:* Precession electron diffraction was invented by Vincent and Midgley exactly 30 years ago and recently ushered its golden era because of the developments of fast direct electron detectors, fast electron beam precession units, advanced processing algorithms and automated instrument control and alignments. Our workshop is targeted to be a forum for relevant researchers to exchange their experience and share their insight on new methods and applications using precession-assisted 4D-STEM and 3D-ED techniques. Part of the presentations will showcase the recent results and further potentials of the recently launched Tescan Tensor STEM platform towards this direction. The workshop is free of charge for participation with a limited capacity. Some short slots (3-5 mins) are spared as flash talks for registered participants to introduce their research results or describe their problems in order to foster collaboration with other participants using the techniques discussed here. Practical demos of Tensor STEM instrument and LiberTEM software package will also be presented.

*Web address:* [https://er-c.org/index.php/conferences/4dstem\\_and\\_3ded/](https://er-c.org/index.php/conferences/4dstem_and_3ded/)

- 3DED workshop at the 9th International Conference on Metal-Organic Frameworks and Open Framework Compounds, 14 July 2024, Singapore

*Number of participants:* ~180

*Level of involvement of SIG in the activity:* SIG4 members involved into the organization and teaching

*ECA Individual Members registered with the SIG involved in the organizing committee:* yes

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed* (SIG logo on the web page/leaflets): No

*Sponsored by ECA* (Yes/ No)? no, not applied for

*Short description:* Three-dimensional electron diffraction (3DED) is a powerful method for structure determination of submicron-sized crystals. The technique overcomes the fundamental drawback of single crystal X-ray diffraction (SCXRD), which requires sufficiently large crystals. Due to recent developments in 3DED hardware and software as well as expanding accessibility of the method, an increasing number of porous crystalline materials, such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), have been determined by 3DED.

This workshop is intended for those who wish to learn the advantages of 3DED and how to apply them for research of MOFs, COFs, and other small molecule crystal structures. The theory of electron diffraction and demonstration of 3DED methods for structure determination of porous materials will be presented in the workshop. Although theoretical background will be briefly reviewed at the beginning of the course, prior knowledge of crystal structures and basic crystallography is highly encouraged for participants in order to benefit most from the school. Researchers from all related fields are welcome to join.

*Web address:* <https://mof2024.mrs.org.sg/pre-conference/>

- ElCryS24 : Electron Crystallography School 2024: "All you ever wanted to know about 3D ED", 24 - 26 August 2024, Padua (Italy), satellite to ECM34

*Number of participants:* 35

*Level of involvement of SIG in the activity:* SIG4 members involved into the organization and teaching

*ECA Individual Members registered with the SIG involved in the organizing committee:* yes

*ECA Individual Members registered with the SIG involved as lecturers:* yes

*SIG endorsed* (SIG logo on the web page/leaflets): yes

*Sponsored by ECA* (Yes/ No)? no, not applied for

*Short description:* International Union on Crystallography (IUCr), IUCr Commission on Electron Crystallography, Special Interest Group for Electron Crystallography (SIG4) of the European Crystallographic Association (ECA) and Italian Crystallographic Association (ICA) are organising "Electron Crystallography School 2024" (ElCryS24) as a satellite event to the 34th European Crystallographic Meeting (ECM34), held in Padua, Italy. The school will take place right before ECM34, on 24 - 26 August 2024 in the Department of Geoscience in Padua.

The interest in electron diffraction has significantly increased in the last ten years in parallel with the automation of routines for data collection, usually performed with a transmission electron microscope. The long-standing issue of multiple scattering (dynamical effects) typical of zone-oriented patterns is significantly mitigated by the possibility to perform three-dimensional, single-crystal-like data acquisitions. This protocol, generally referred as three-dimensional electron diffraction (3D ED) or microcrystal electron diffraction (MicroED), allows for the acquisition of structural data from single crystals with size of few tens of nanometers, regardless of the nearby presence of other phases. Therefore, 3D ED has been successfully used for the structure determination of several dozen of new inorganic and organic compounds that were previously considered intractable by X-ray diffraction methods. Moreover, electron diffraction is more sensitive to light atoms, ionic charges, and the absolute structure in chiral compounds. Such potential can be fully exploited through a careful structural refinement that considers the residual dynamical effects.

Ten lecturers have been selected among the most prominent European experts in electron crystallography. Students will benefit from frontal lectures about theory and practice of electron diffraction as well as from practical sessions during which they will familiarize themselves using their own laptop with a complete workflow of data processing, from raw electron diffraction data up to structure refinement. The main idea behind the school is to bring students in direct contact with the very people developing software for electron diffraction. We believe this is the best way to create a beneficial interaction between researchers involved in the development of new methodologies and researchers interested in specific material characterization.

*Web address:* <https://elcrys24.sciencesconf.org/>

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## List of plenary / invited / teaching lectures of individual SIG members.

Invited lecture: *"In situ 3DED in gas and liquid environments for following structural evolutions during reactions"*, 20th International Microscopy Congress, September 2024, South-Korea, **Joke Hadermann**

Invited lecture: *"Revealing Invisible: Analysis of MOF and COF Nanocrystals by 3D Electron Diffraction"*, the 9th International Conference on Metal-Organic Frameworks and Open Framework Compounds, 15-19/07/2024, Singapore, **Zhehao Huang**

Invited lecture: *"Analysis of Structure and Properties of Porous Materials Using 3D Electron Diffraction"*, the 45th International Conference on Coordination Chemistry, July 28 – Aug 3 2024, USA, **Zhehao Huang**

Keynote lecture: *"Structure elucidation of complex materials by three-dimensional electron diffraction"*, SMARTER Crystallography Meeting 8, 22-25/09/2024, Portugal, **Zhehao Huang**

Invited lecture: *"Analysis of the fine structure of porous materials using three-dimensional electron diffraction"*, the 2<sup>nd</sup> World Materials Conference, 8-11/07/2024, China, **Zhehao Huang**

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## Current List of SIG4 officers

Chair: Tatiana Gorelik, [tatiana.gorelik@helmholtz-hips.de](mailto:tatiana.gorelik@helmholtz-hips.de)

Vice Chair: Stéphanie Kodjikian, [stephanie.kodjikian@neel.cnrs.fr](mailto:stephanie.kodjikian@neel.cnrs.fr)

Secretary: Lukáš Palatinus, [palat@fzu.cz](mailto:palat@fzu.cz)

Webpage administration: Tim Gruene, [tim.gruene@univie.ac.at](mailto:tim.gruene@univie.ac.at)

Mailing list administration: Jerome Pacaud, [jerome.pcaud@univ-poitiers.fr](mailto:jerome.pcaud@univ-poitiers.fr)