

SIG4 activity report September 2024-August 2025

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), co-editor Zeitschrift für Kristallographie (De Gruyter Brill)

Joke Hadermann: co-editor of Acta Cryst B (IUCr), Journal of Solid State Chemistry (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)

Organization of ECM

SIG4 representative in the organizing committee of ECM35 Poznan / Lviv 2025 – Sergi Plana Ruiz

List of MSs @ECM35 organized / proposed by SIG:

MS37 – Advanced and new techniques to study inorganic materials (1.D) Chairs: Mariana Klementova (FZU-CAS, Prague, Czech Republic), Andrew Stewart (Univ. College London, United Kingdom)

MS7 – Electron diffraction of macromolecules (1.E) Chairs: David Owen (Diamond LS, Didcot, United Kingdom), Xiaodong Zou (Stockholm Univ., Sweden)

MS15 – Inorganic crystal structure investigation using electron diffraction (1.A) Chairs: Stéphanie Kodjikian (Institut Néel, Grenoble, France), Louisa Meshi (Ben-Gurion Univ. Negev, Beersheba, Israel)

MS40 – New developments in electron diffraction (1.D) Chairs: Paul Klar (Univ. Bremen, Germany), Ute Kolb (Univ. Mainz, Germany)

Keynote

A Journey to the Nanoscale through Electron Diffraction – Sergi Plana Ruiz (Univ. Rovira i Virgili, Tarragona, Spain) – replacing Yasar Krysiak

Invited talks:

MS37_01 / invited speaker: Direct imaging of beam-sensitive inorganic materials using 2D and 4D scanning transmission electron microscopy – Peter Nellist (Oxford Univ., United Kingdom)

MS7_01 / invited speaker: Counting and filtering macromolecular electron diffraction data – Max Clabbers (Aarhus Univ., Denmark)

MS7_02 / invited speaker: Developing electron diffraction methods to probe oxidation states in metalloenzymes – Laura Pacoste (Stockholm Univ., Sweden)

MS15_01 / invited speaker: Scanning electron crystallography powered by machine learning – Yevgeny Rakita (Ben-Gurion Univ. Negev, Beersheba, Israel)

MS15_02 / invited speaker: Advanced electron diffraction techniques for functional material structural analysis – Christophe Lepoittevin (Institut Néel, Grenoble, France)

MS40_01 / invited speaker: Experimental charge densities of organic nanocrystals from 3D electron diffraction Paulina Dominiak (Univ. Warsaw, Poland)

MS40_02 / invited speaker: Crystal structure determination and refinement from serial precession electron diffraction Sergi Plana-Ruiz (Univ. Rovira i Virgili, Tarragona, Spain)

MS41_01 / invited speaker: Electron Pair Distribution Function analysis in the scanning TEM for probing nanoscale heterogeneity in amorphous and crystalline polymers and metal-organic frameworks – Sean Collins (Univ. Leeds, United Kingdom)

MS20_01 / invited speaker: Aperiodic crystallography from 3-dimensional electron diffraction using kinematic and dynamical approaches – Gwladys Steciuk (Univ. Lorraine, Metz, France)

SIG4 webpage and mail list

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

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

Mail list administrators are

Jérôme Pacaud jerome.pacaud@univ-poitiers.fr

Andrew Stewart andy.stewart@ucl.ac.uk

New subscriptions: 10

Messages 15 (Position offers 4; workshop announcement 4; SIG (medals, report) 7)

Fortunately, there was no spam subscription this year.

Prizes sponsored/coordinated

SIG4 distinguished publication award 2025 (for 2024) will be announced at the ECM35, the chair of the prize committee is Sergi Plana Ruiz.

Organization of dedicated schools / workshops

- Two 48th Ad Hoc Workshop on Jana2020 Electron diffraction, Prague, Part I October 21-22, Part II October 24-25 2024

Number of participants: 14 (Part I) and 14 (Part II)

Level of involvement of SIG in the activity: SIG4 members in the organization and teaching (Lukas Palatinus, Mariana Klementova, Gwladys Steciuk, Petr Brazda)

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

- Theme days “RX, neutrons, electrons: similarities and differences in diffraction and imaging” (13-14 November 2024, Grenoble, France)

Number of Participants: 50

Level of involvement of SIG in the activity: organization (S. Kodjikian, C. Lepoittevin), and lecturing (P. Boullay, D. Jacob, D. Housset)

ECA Individual Members registered with the SIG involved in the organizing committee: yes (Stéphanie Kodjikian, Christophe Lepoittevin)

ECA Individual Members registered with the SIG involved as lecturers: yes (Philippe Boullay, Damien Jacob, Dominique Housset)

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

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

Short description: seminars

Web address: <https://neel.cnrs.fr/actualites/journees-rime-reciprocs>

- International School of Crystallography: 60th Course: Electron Crystallography, Erice, Italy 30 May - 7 June 2025

Number of participants: 40

Level of involvement of SIG in the activity: SIG4 member in 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): yes

Short description: In recent years, electron crystallography has undergone a tremendous development from a niche technique to an established method of structure analysis standing in line with x-ray and neutron crystallography. The technique continuously gains in popularity, covering new applications and developing new methodologies, thus requiring new experts with very specialized interdisciplinary knowledge of electron scattering and crystallography.

Consequently, the primary focus of the school is to provide comprehensive education on the workflow of the 3D ED/MicroED technique, covering various aspects of data collection, processing, and structure analysis. Students will acquire hands-on experience in structure analysis using electron diffraction data, thereby gaining a broad perspective on adjacent experimental and theoretical methods. With a diverse range of examples, we will explore all materials classes, including inorganic, organic and macromolecules. Additionally, we will demonstrate approaches for addressing unconventional structural problems.

A pivotal topic of the school will be the physics of electron scattering, including its implications for structure analysis, such as dynamical refinement. A central part of the program will be fundamental crystallographic education including the modern crystallographic methods of structure analysis and relevant software, which will be covered explicitly in dedicated lectures and tutorials.

In addition to teaching state-of-the-art crystallographic structure analysis with electrons, the program will explore emerging topics in electron scattering that may shape the future of structural science. The scope extends beyond 3DED to cover future trends such as 4D-STEM, ptychographic methods, structural dynamics and the analysis of disordered and amorphous structures with electrons.

Additionally, the school will benefit from the synergy with the Quantum Crystallography School running in parallel, with several lectures shared between the two schools. This will offer a unique opportunity to explore interdisciplinary applications of crystallography in quantum science and structural research.

Web address: <https://crystalerice.org/2025/welcome.php>

- Practical course "3D electron diffraction" (Grenoble, France, 18-20/06/2025)

Number of participants: 4

Level of involvement of SIG in the activity: 3 SIG4 members in the organization and teaching (Dominique Housset, Stéphanie Kodjikian, 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, with alternation of demonstrations and manipulations on TEM, and tutorial sessions on computer.

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

- Workshop on 3D ED organized as side event of the SCCM25 (31st Slovenian-Croatian Crystallographic Meeting 2025) at the Faculty of Chemistry and Chemical Technology, University of Ljubljana Slovenia the 18th of June 2025.

Level of involvement of SIG in the activity: SIG member Mauro Gemmi involved as a teacher.

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

Short description: A one day course on 3D ED with direct demonstration of data collection at a recently installed Rigaku Synergy ED electron diffractometer and of data analysis of the collected data. Number of participants: 25 students.

- Laboratory experience for high-school students (from Gymnasium Thun, Switzerland) at the Department of Chemistry, University of Copenhagen, Denmark. 2nd July 2025.

Number of participants: 7 students.

Level of involvement of SIG in the activity: SIG member Arianna Lanza involved as organizer and teacher.

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

Short description: A one-day practical experience for high-school students about synthesis and structure characterization of active porous materials for absorption of gases. The students have synthesized the materials in 2 different ways and observed the colour changes upon sorption and desorption of water and ammonia. Preliminary phase analysis was performed with PXRD. 3D ED was used to solve the structure of the absorbed and desorbed compounds. Demonstration of data collection at two different temperatures and structure solution.

- Invited seminar – “Electron Crystallography for Materials Science & Nanotechnology”, 13th May 2025, ICMAB-CSIC, Bellaterra, Catalonia. Link: <https://www.youtube.com/watch?v=oaszkd-Fd4k&t=2848s>
- 36th ECA Lunch webinar from 24th April 2025: Dr. Alke Meents and Dr. Paul Klar: Structure determination with 3 MeV electron crystallography <https://www.youtube.com/watch?v=w74IG8SOM98>

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

Invited lecture – “*Highlights from the NNF-CHEM infrastructure Center for Electron Diffraction*”, within the Seminar “*Micro electron diffraction: impact in protein science and chemistry*” organized by Prof Leila Lo Leggio and JSPS Stockholm-Alumni Club Denmark, 13th February 2025, University of Copenhagen, Denmark, Arianna Lanza

Current List of SIG4 officers

Chair: Tatiana Gorelik, t.gorelik@fz-juelich.de

Vice Chair: Stéphanie Kodjikian, stephanie.kodjikian@neel.cnrs.fr

Secretary: Sergi Plana Ruiz, sergi.plana@urv.cat

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