



## Activity report of the European Crystallographic Association

April 2024 – March 2025

### Scope of activities

ECA has continued supporting the crystallographic community in Europe and beyond, especially through its networking activities, conferences, schools, communication, prizes, awards and bursaries. It relies on seventeen Interest Groups either focused on a particular branch of the field or on networking activities.

ECA Interest Groups at the end of the reporting period:

#### *Special Interest Groups*

- SIG-01 Macromolecular Crystallography
- SIG-02 Quantum Crystallography
- SIG-03 Aperiodic Crystallography
- SIG-04 Electron Crystallography
- SIG-05 Mineralogical Crystallography
- SIG-06 Instrumentation and Experimental Techniques
- SIG-07 Molecular Interaction and Recognition
- SIG-08 Powder Diffraction
- SIG-09 Crystallographic Computing
- SIG-11 Extreme Conditions
- SIG-12 Materials Science
- SIG-13 Molecular Structures and Chemical Properties
- SIG-14 Dynamics, Disorder, Diffuse scattering
- SIG-15 Crystallography in Art and Cultural Heritage (newly approved August 2024)

#### *General Interest Groups*

- GIG-01 Young Crystallographers
- GIG-02 Senior Crystallographers
- GIG-03 Education in Crystallography

The Interest Groups were involved in planning the scientific program of the European Crystallographic Meeting 34 in Padova, Italy, organization of their own activities, such as poster prizes and schools with focus on their areas. They were also active in preparation of the upcoming ECM35 in Poznan/Lviv in 2025. Several of the ECA Interest Groups have elected their new officers and their current representatives are shown at the ECA web pages <https://ecanews.org/current-interest-groups/>.

## Conferences and Schools

ECA is involved in two flagship events – the European Crystallographic Meeting and the European Crystallographic School.

### European Crystallographic Meeting 34, Padova, Italy, 26-30 August 2024

The ECM34 congress (<http://ecm34.ecanews.org>) welcomed more than 800 participants who contributed in 43 microsymposia spanning from quantum crystallography over applications in material and biological sciences to teaching and crystallography in art, accompanied by about 700 posters. The plenary lectures were given by Kristina Djinovic on the molecular architecture of muscles and by Jonathan Wright providing insights into imaging single crystals in powder samples. The most significant developments in the key directions of instrumentation, computational tools and application of crystallographic approaches in various branches of research were presented in 16 keynote lectures. The social program offered amongst others the Science Slam, a great concert of classical music in Palazzo Liviano, a public lecture “Einstein and Me” by Gabriella Greison, a students’ mixer, and an unusual experience in the form of a conference dinner in one of the historical city squares.

ECM34 was complemented by seven satellite events, including the European Young Crystallographers Satellite Meeting or the special event Crystallography in School promoting teaching of crystallography with school science teachers. The organizing committee chaired by Gilberto Artioli and Giuseppe Zanotti with the help from the chairs and co-chairs of the individual microsymposia managed to prepare a great event with exciting topics, excellent speakers, and plenty of space for social and scientific interactions. The crystallographic song “A musical account of a rather unfortunate trainee crystallographer” by Bill Clegg on the music by Wolfgang Amadeus Mozart performed in the Science Slam and for great success also during the closing ceremony was a treat to all crystallographers enjoying apart from science also good music and fun.



Lecture of Prof. Mariusz Jaskolski at ECM 34 – the 2024 Max Perutz prize winner

Five crystallographic prizes have been awarded during the Meeting. The Max Perutz Prize to Prof. Mariusz Jaskólski, Adam Mickiewicz University in Poznań, accompanied with his lecture “A path paved with crystals”, the Erwin Felix Lewy Bertaut Prize to Daniel Mazzone, Paul Scherrer Institute, Villigen, and the Alajos Kálmán Prize to Piero Macchi, Politecnico di Milano. Two newly established prizes have been awarded for the first time: The Lodovico Riva di Sanseverino prize in recognition of notable contributions to the dissemination of

crystallography in the field of education at all levels to Claire Murray, Freelance Scientific Researcher in Germany and the George M. Sheldrick prize to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences to Marta Morana, University of Florence.

Eleven poster prizes, supported by companies, IUCr Journals, CCDC and others, appreciated the best poster presenters, in specific fields of research, instrumentation development or at the start of their career.

### **Preparations for the European Crystallographic Meeting 35, Poznań/Lviv, 25-29 August 2025**

The ECA Executive Committee and SIG and GIG representatives have been assisting the local organizing committee and the scientific program committee of ECM35 to ensure success of this event marked by an uneasy political and security situation in Europe. ECA has supported the idea of the ECM originally planned in Ukraine and being moved to Poland, as a rescue solution offered by the colleagues from the Adam Mickiewicz University in Poznań. We are glad to witness the organizers from Lviv and Poznań joining in their effort to prepare the next ECM congress.

### **9<sup>th</sup> European Crystallography School, Nancy, 24-30 June 2024**

ECS9 (<https://ecs-9.event.univ-lorraine.fr/>) was focused on improving crystallography skills: from basic structure analysis to understanding of chemical bonds, bonding interactions and structure-properties relationships in materials. The main sections were dealing with (i) An introduction to X-Ray Diffraction (XRD) theory, (ii) Structure determination and analysis, (iii) Packing and interaction analyses, (iv) Using aspherical models of the electron density distribution, and (v) Crystallography under constraints. The school was attended by 62 participants from 22 countries. The School was supported by 16 sponsors and enabled hands-on computational training, discussions and informal exchanges between lecturers and attendees. Two posters of the participants were awarded prizes sponsored by CCDC and CRM2.

## **Prizes and awards**

In 2024 the portfolio of the ECA prizes has been extended by two new awards. The Lodovico Riva di Sanseverino prize in recognition of notable contributions to the dissemination of crystallography in the field of education was for the first time awarded in connection with ECM34 in Padova (see above) as well as the first award of the George M. Sheldrick prize to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences. Both Prizes are accompanied by a monetary reward and a lecture presented by the awardee at the ECM meeting.

### **Current portfolio of ECA prizes**

Max Perutz Prize (awarded each ECM year), Erwin Félix Lewy Bertaut Prize (awarded by ENSA and ECA – agreed schedule), Alajos Kálmán Prize (awarded each ECM year), Lodovico Riva di Sanseverino Prize (awarded once in three years, in an ECM year), George M. Sheldrick Prize (awarded each ECM year).

## Bursaries and grant support

ECA also supports other conferences and schools with a focus on crystallography and an international impact, mainly in Europe. For this purpose, each year grants are awarded based on individual applications in two rounds. In 2024-2025 ECA supported 3 conferences, 1 workshop and 5 schools with a total grant support of € 11,050.

- **20th BCA/CCG Intensive Teaching School in X-ray Structure Analysis**, 29 March – 5 April 2025, Durham University, UK
- **Hot Topics in Contemporary Crystallography 6 – HTCC6 workshop**, 7-12 April 2024, Dubrovnik, Croatia
- **60th ERICE School - Electron Crystallography**, 30 May – 7 June 2025, Ettore Majorana Foundation and Center for Scientific, Culture – Erice (TP) – Italy
- **61st ERICE School - Quantum Crystallography**, 30 May – 7 June 2025, Ettore Majorana Foundation and Center for Scientific, Culture – Erice (TP) – Italy
- **59th course of the ISCoC: “Real materials in information era”**, 31 May - 8 June 2024, Erice, Italy
- **30th Croatian-Slovenian Crystallographic Meeting (CSCM30)**, 12-16 June 2024, Veli Lošinj, Croatia
- **The Zurich School of Crystallography 2024 – Bring Your Own Crystal**, 17-29 June 2024, Zürich, Switzerland
- **European Powder Diffraction Conference (EPDIC18)**, 30 August - 2 September 2024, Padova, Italy
- **6th International Symposium on Halogen Bonding (ISXB6)**, 20-25 October 2024, Dubrovnik, Croatia
- **9th European Crystallography School (ECS9)**, 24-30 June 2024, Nancy, France

The Association also provided 12 travel grants to young early career researchers (350 € each) to attend the ECM34 in 2024 and to prize winners. The annual European Crystallographic School, in 2024 ECS 9 in Nancy (France), was supported by € 3,000. Next to these activities in 2024 ECA supported education activities in Africa with € 1,000.

In 2024 the direct financial support to women participating in crystallographic conferences or courses was started, using the Women-in-Crystallography fund; in total € 1.750 was awarded to four young female researchers.

## ECA Lunchtime Webinars

Since June 2021 the young crystallographers of ECA have run the ECA Lunchtime Webinars focusing on the current and hot topics across the whole field of crystallography. Eight monthly webinars were held in the past period regularly attracting 30-60 followers online (the recordings are available online at [https://ecanews.org/education/eca-lunch-webinars\\_past-events/](https://ecanews.org/education/eca-lunch-webinars_past-events/)):

Webinar 28: **Ross John Angel**, *How to evaluate published high-pressure experiments*, 11 April 2024

Webinar 29: **Gianluca Iori**, *BEATS: Synchrotron computed microtomography for the Middle East*, 6 June 2024

Webinar 30: **Kludia Hradil**, *Introducing SIG15: Crystallography in Preserving, Exploring and Communicating Cultural Heritage*, 10 October 2024

Webinar 31: **Arkadiy Simonov**, *Seeing structure of disordered single crystals through the lens of diffuse scatterings*, 14 November 2024

Webinar 32: **Dietmar Stalke**, *Basic chemical concepts challenged by experimental charge density*, 5 December 2024

Webinar 33: **Sofia Trampari**, *Collecting the best data for Macromolecular Crystallography with HPC detectors*, 23 January 2025

Webinar 34: **Erhard Irmner**, *Crystallography in School?!*, 20 February 2025

Webinar 35: **Alessia Bacchi**, *From liquid ingredients to crystalline smart materials*, 27 March 2025

## Distinguished Lectures on Quantum Crystallography and Complementary Fields

SIG-02 of ECA has continued the very successful series of online lectures “Distinguished Lectures on Quantum Crystallography and Complementary Fields”, which represent a valuable effort to broaden the knowledge and applicability of quantum crystallography across many other fields of science

(<https://qcrwebinar.chem.uw.edu.pl/>)

Lecture 38: **Martin Rahm**: *The Electron Density: a Fidelity Witness for Quantum Computation*, April 18, 2024

Lecture 39: **Peter Baum**: *Attosecond and femtosecond electron microscopy*, April 18, 2024

Lecture 40: **Nicola Clauser**: *Joint refinement of diffraction data (but not only): a short story*, October 3, 2024

Lecture 41: **Huibo Cao**: *Chirality and magnetic symmetry*, October 3, 2024

Lecture 42: **Sajesh Thomas**: *Chemical Applications of X-ray Quantum Crystallography*, December 5, 2024

Lecture 43: **Sarah Guerin**: *Rational Design of Complex Electromechanical Phenomena in Molecular Crystals*, December 5, 2024

Lecture 44: **Louis Massa**: *Energy formalism of an X-ray electron density of large biological molecules*, January 16, 2025

Lecture 45: **Paul Popelier**: *The Relative Energy Gradient (REG) Method or How to Compute Chemical Insight*, March 6, 2025

Lecture 46: **Sarah Price**: *Organic Crystal Structure Prediction: What is Needed for Confident Prediction of Polymorphs?*, March 6, 2025

## ECA Governance

In 2024 the election term of the Executive Committee ended, and a new Committee was elected by the ECA Council in Padova. The achievements of the outgoing Executive Committee were appreciated by the Council and some Committee members have been re-elected to their new roles.



Executive Committee members, outgoing and newly elected, Padova, August 2024

## Executive Committee members (after 2024 elections)

President – Dr. Arie van der Lee (Université de Montpellier)  
 Immediate past president – prof. Marijana Đaković (University of Zagreb)  
 Vice-president – Dr. Jan Dohnálek (Institute of Biotechnology AS CR, Vestec near Prague)  
 Secretary – Dr. Andy Maloney (Cambridge Crystallographic Data Centre)  
 Treasurer – prof. Antonia Neels (Swiss Federal Laboratories for Materials Science and Technology, Dübendorf; University of Fribourg)  
 Education coordinator – Dr. Maria José Sanchez Barrena (Instituto de Química Física “Blas Cabrera”, Madrid)  
 Officer (SIG, GIG, IM) – prof. Chiara Massera (University of Parma)  
 Officer (National members) – assoc. prof. Katarzyna Jarzemska (University of Warsaw)  
 Officer (Grants) – Dr. Klaudia Hradil (TU Wien)  
 Officer (Webmaster) – Dr. Andrea Ienco (Istituto di Chimica dei Composti Organo-Metallici, Sesto Fiorentino)



ECA Executive Committee, Montpellier, March 2025

## Council meeting

ECA Council met at the occasion of the ECM34 congress in Padova on 27 and 29 August 2024. The following key decisions/changes were approved by voting, apart from the annual reports:

- ECA webmaster is newly an officer of the Executive Committee
- Election of the new Executive Committee for the term 2024-2027 (see above)
- Approval of bid for organization of ECM37 (2028) in Athens, Greece
- Approval of bid for organization of ECS11 (June 2026) in Stockholm, Sweden
- Increase of membership fees

Other issues discussed based on reports and proposals (without binding decisions) included: individual membership visibility, meetings of individual members at ECMs, and improved descriptions of prizes on ECA webpages.

## Executive Committee meetings

The Executive Committee of ECA met three times during the reporting period to discuss all ECA matters, including reporting and planning of events, grant applications, changes in organization and finances.



Online meeting, 7 June 2024

The main agenda points of this online meeting included proposals to increase the membership fees of individual members and corporate and associate members, Darmstadt funds, last preparations for ECM34 in Padova, progress of ECM35 preparations, GIG-03 Women in Crystallography activities, and increase of ECM travel grants.

Padova, 26 & 30 August 2024

The Executive Committee met twice at the occasion of ECM34 in Padova. The main discussed points were the national memberships of Algeria, Morocco, Egypt, Tunisia, Romania, Belarus and Estonia, increase of support to the ECS schools, transfer of Darmstadt funds, preparations of ECM35 Lviv/Poznan in 2025, reports, progress reports and bids for ECS organization, communication with SIGs and GIGs, and publicity of ECA at ECMs. Details of key points to be presented to the ECA Council were agreed, including the increase of membership fees for individual and corporate members. The second meeting of the newly elected Executive Committee expressed gratitude to the leaving members, established the portfolios of new members or members in their new roles, and focused on the transfer of responsibilities between the committee members.

Montpellier, 9-11 March 2025

A primary focus of the meeting was the ECA's core activities: ECMs and (ECSs, as well as the association's support for young crystallographers through travel grants and financial assistance for schools, workshops, and outreach initiatives. The organizers of ECM34 (Padova, Italy) presented a near-final report on the congress's preparations, while the organizers of ECM35 (Lviv-Poznan) provided an update on their progress since August 2024. The Executive Committee discussed with the ECM35 organizers how to best organize a tribute to George M. Sheldrick. Additionally, updates were provided on the forthcoming ECS10 in Ohrid, North Macedonia, and the ongoing planning for ECS11 in Stockholm, Sweden. The committee also explored ways to enhance and expand support for young crystallographers.

## New activities

### Video series Women in Crystallography

An effort to present inspiring stories of women in the field has materialized into the first five videos of a new series Women in Crystallography, originated by GIG-03 of ECA and supported by The Royal Society of Chemistry (<https://www.youtube.com/@ECA-Crystal/videos>):

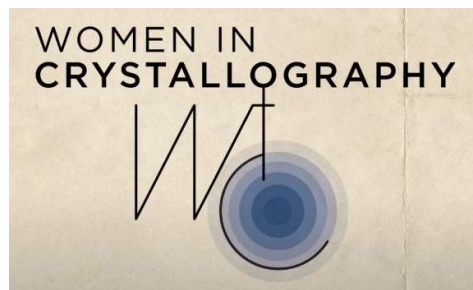
**Shanti Deemyad**, *Journey Through the Quantum Realm: My Path as a High-Pressure Physicist*

**Julia Contreras-García**, *Be Proactive*

**John R. Helliwell**, *Women in science & crystallography*

**Anna Pakhomova**, *Under high pressure: crystallographer, beamline scientist, and mum*

**Bart Kahr**, *Did the crystallographic content of late nineteenth century kindergarten play a role in the explosion of research into the architecture of crystals... in particular the spectacular rise of women?*



### Video contest for high school students

The GIG-03 initiated the First European Video Contest with support of ECA and CCDC, focused on high school students demonstrating their abilities in crystal growing and interest in crystallography. The competition attracted significant attention, and the first three students were awarded prizes in two age categories. The winners' videos are available here <https://ecanews.org/blog/2024/07/26/results-of-the-first-european-crystallography-video-contest/>.

### 1st Kenyan Crystallization Contest at School

The first Kenyan Schools Crystallography Competition was held with the support of ECA, introducing secondary school students to crystallography and scientific research. The competition was structured as a scientific conference with the award ceremony at the Chiromo campus of the University of Nairobi on 25 January 2025. More information can be found at the competition website: <https://kenyancrystallizat.wixsite.com/blog>.



### Satellite meeting Crystallography in School

A new type of satellite meeting of ECM34 in Padova called Crystallography in School was organized by GIG-03, a half-day workshop focused on sharing teaching modules and on good practices in crystallography-related subjects in school.

### Outlook for the upcoming period

The calendar of the ECA-related future events has been extended by the newly approved organization of the European Crystallographic School 11 in Stockholm, June 21-27, 2026, and of ECM37 in Athens, August 2028.

### Upcoming events of ECA

ECS10, Ohrid, Northern Macedonia, 22-27 June 2025  
 ECM35, Poznań/Lviv, Poland/Ukraine, 25-29 August 2025  
 ECS11, Stockholm, Sweden, 21-27 June 2026  
 ECM36, Prague, Czech Republic, August 2027  
 ECM37, Athens, Greece, August 2028



# European Crystallographic Association

## Signatures page

2025



The undersigned hereby declare that they have read and approved the contents of the present report.

### ECA Executive Committee (2024-2027)

Arie van der Lee (President)

Jan Dohnálek (Vice-President)

Marijana Đaković (Past-President)

Andrew Maloney (Secretary)

Antonia Neels (Treasurer)

Maria José Sanchez Barrera (Education Coordinator)

Chiara Massera (Officer - SIGs, GIGs, IMs)

Katarzyna Jarzemska (Officer - National Members)

Kludia Hradil (Officer -Grants)

Andrea Ienco (Officer - Webmaster)