

Activity report of the European Crystallographic Association

April 2023 – March 2024



A year without a European Crystallographic Meeting but not without activities

European crystallographers meet usually in years when the International Union for Crystallography does not organize its triennial congress. 2023 was such a year when the worldwide crystallographic community gathered in Melbourne, Australia. The ECA Council meeting was held remotely in two different sessions to ensure as high an attendance as possible, on the 20th and 22nd of September 2023. Meetings of the Executive Committee were organized remotely just before the Council Meeting on the 11th and 12th of September 2023 and another one in Poznań, Poland, from the 2nd to the 4th of February 2024. The webinar series organized by ECA's Special Interest Group 2 (Quantum Crystallography) jointly with the IUCr Commission on Quantum Crystallography and ECA's lunchtime webinars organized by the General Interest Group 1 (Young Crystallographers) continued to take place at regular intervals throughout the year. One prize was jointly awarded by ECA and the European Neutron Scattering Association: the twelfth Erwin Félix Lewy Bertaut Prize went to Matilde Saura-Múzquiz (Departamento de Física de Materiales of the Universidad Complutense in Madrid, Spain). The eighth European Crystallographic School took place in Berlin from the 19th to the 23rd of June 2023.

Council Meeting (20th, 22nd of September 2023)

A considerable part of the business at ECA Council Meetings naturally concerns the planning of future European Crystallographic Meetings, and Councillors receive progress updates on the planning of upcoming meetings as well as the opportunity to vote for the location of future ECMs. Preparations are well underway for ECM34, which is scheduled to take place in Padova, Italy, from the 26th – 30th August 2024 (more information is available on the conference website: <https://ecm34.ecanews.org/>). It should be noted that EPDIC18, the European Powder Diffraction Conference, will be held immediately after ECM34 at the same venue (<https://www.epdic18.org/>).

Due to the ongoing conflict in Ukraine, where ECM35 was due to be held in 2025, a proposal was made by the Polish Crystallographic Association in collaboration with ECM35 organisers and other Ukrainian colleagues to move the location of the conference to Poznań, which was approved by the Council. A bid from Czech colleagues to hold ECM36 in 2027 in Prague (at the same location as the 25th IUCr Congress in 2021) was also presented and approved.

The topic of prizes of the ECA was also discussed in detail. The ECA awards a number of prizes at its meetings, including the Max Perutz Prize (awarded in recognition of meritorious achievements in any branch of crystallography), the Erwin Félix Lewy Bertaut Prize (awarded to a young scientist in recognition of notable experimental, methodological, or theoretical contributions to the investigation of matter using crystallographic or neutron scattering methods), and the Alajos Kálmán Prize (awarded by the Hungarian Chemical Society in recognition for outstanding scientific contributions in the field of structural sciences). At the Council meeting in September proposals were heard and approved for the incorporation of two new prizes related to ECA: the George M. Shelbrick Prize (awarded to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences) and the Lodovico Riva de Sanseverino Prize (awarded in recognition of notable contributions to the dissemination of crystallography in the field of education at all levels). More information is available online: <https://ecanews.org/prizes/>.

Finally, of interest to younger members of the crystallographic community, the ECA Council heard the report on the 8th European Crystallographic School (ECS8), which took place in-person in Berlin, Germany, in June this year. European Crystallographic Schools combine lectures and hands-on tutorials to provide attendees a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater to a broad range of interests. ECS9 will take place during 2024 in Nancy, France (from the 24th – 30th June 2024), and a successful bid takes ECS10 to Lake Ohrid, North Macedonia, in 2025. For further information on the ECS, please visit <https://ecanews.org/european-crystallography-school/>.

Executive Committee Meetings (11th, 12nd of September 2023; 2nd – 4th of February 2024)

Much of the work of the first remote ExComm meetings was devoted to the preparation of the Council meeting which followed 10 days later. The second ExComm meeting, usually called Winter Meeting, was held at the venue of ECM35, in Poznań in Poland. ExComm usually holds its Winter Meeting at the venue of a future ECM, approximately one and a half year before the start of the congress. ExComm had the chance to visit the Poznań Congress Center, where the congress is envisioned to be held, and to speak not only with the main local organizers Grygoriy Dmytriv and Maciej Kubicki, but also with people from Adam Mickiewicz University (AMU), the professional Congress Organisation (AMU Foundation), and the Poznań Convention Bureau.

Giuseppe Zanotti and Gilberto Artioli from the local organizing committee of ECM34 in Padova, Italy, were remotely present to discuss the progress in the organization of this congress. The proposed fees for ECM34 are higher than previous ECMs due to economic challenges particularly around inflation in Italy and expense of the venue, but are comparable to those of similar congresses. Eight satellite meetings are planned so far. Registration and submission of abstracts have started in February 2024. Radomír Kužel, chair of the local organizing committee of ECM36, to be held in Prague, Czech Republic, in 2027, was also remotely present. The conference centre in Prague is the same as for the IUCr congress in 2021.



Group photo of ECS8 held in Berlin (June 2023). Photo by Manfred Weiss.

Reports from the organizers of the last European Crystallographic School, ECS8 in Berlin, and the next Schools, ECS9 in Nancy, France (24-30 June 2024), and ECS10 in Ohrid, North Macedonia (22-29 June 2025), were received. Plans for future ECSs (ECS11, ECS12) were considered.

ECA finances were discussed extensively: it was decided to increase the part of the budget which is allocated to the support of schools, workshops and congresses, in particular for ECA's own European Crystallographic Schools.

ECA's prizes were discussed as well and the proposed prize committees which will stand for a period of six years were approved. The call for nominations for the five prizes was made early February 2024.

ECA's General Interest Group 3 (GIG-03: Education in Crystallography) has received a grant from the Royal Society of Chemistry (5k£), for the preparation and dissemination of a series of ten video interviews to celebrate the importance of women in the field of crystallography and science, while, at the same time, raising awareness about the pitfalls and obstacles on the way to reach gender parity in science. The first video will be launched in June 2024. GIG-03 also prepares a Crystallization Video Competition (using a grant obtained from the Cambridge Crystallographic Data Centre) for schoolchildren in different European countries. The aim is to present the winning videos at the next European Crystallographic Meeting in Padova in August 2024.

Electronic archiving of websites of past European Crystallographic Meetings and Schools has continued: currently the websites of ECM18, ECM21, ECM22, ECM23, and ECM27-ECM33 have been made available at

<https://ecmxx.ecanews.org> where xx is the ECM number and those of ECS1–ECS7 at <https://ecsxx.ecanews.org> where xx is the ECS number.

ECA's webinars

European crystallographers continue to meet during ECA's monthly lunchtime webinars, a successful series of on-line seminars covering all sub-disciplines in crystallography and organized by ECA's young crystallographers. Eight lunchtime webinars took place from April 2023 until March 2024:

- 13th April 2023, Claire Murray (UK), *Crystallography for the people*
- 25th May 2023, Clive Oliver (South Africa), *Small molecular and crystal structure changes in MOFs leading to large differences in sorption and thermosolvent properties*
- 29th June 2023, Martina Vrankić (Croatia), *A key purpose of high-pressure research - effect of pressure on structures and functionalities of materials*
- 5th October 2023, Catherine Dejoie (France), *High-resolution X-ray powder diffraction – Application to the study of CO₂ trapping in microporous materials*
- 23th November 2023, Tatjana Barthel (Berlin), *Crystallographic fragment screening at the HZB - Workflow, tools and procedures*
- 25th January 2024, Bill Clegg (UK), *Why do so many crystal structures remain unpublished?*
- 15th February 2024, Sergi Plana Ruiz (Spain), *Liquid phase electron crystallography: The path to electron diffraction from protein crystals at room temperature*
- 14th March 2024 Martin Schmidt (Germany), *Nanocrystalline organic compounds: Crystal structure determination from XRPD and PDF data - What is possible today?*

Another series of webinars, the *Distinguished Lectures on Quantum Crystallography and Complementary Fields*, initiated by ECA's Special Interest Group 2 (Quantum Crystallography) and the IUCr Commission on Quantum Crystallography continued as well: eight webinars took place, usually with two lectures during the same webinar:

- 16th March 2023, Ángel Martín Pendás (Spain), *Is the one-particle approximation biasing our interpretation of real space chemical bonding descriptors? The cases of the Laplacian of the electron density and the electron localization function*
- 16th March 2023, Michele Ceriotti (Switzerland), *Physics-based machine learning of the electron density*
- 5th May 2023, Anders Madsen (Denmark), *Dynamic quantum crystallography: Thermal motion in crystallography seen through a quantum-mechanical looking glass*
- 5th May 2023, Rebecca Nicholls (UK), *Phonon vibrations probed using the electron microscope*
- 1st June 2023, Enrique Espinosa (France), *Topological analysis of the electrostatic potential in molecular systems*
- 1st June 2023, Holger Stark (Germany), *Breaking the ice: Cryo-EM's quest for better resolution and quality*
- 26th October 2023, Simon Grabowsky (Switzerland), *Quantum crystallography for chemical bonding analysis*
- 26th October 2023, F. Matthias Bickelhaupt (The Netherlands), *Covalent interactions: A quantitative molecular orbital picture*
- 16th November 2023, Cherif Matta (Canada), *ATP synthase: More than just a biocatalyst?*
- 16th November 2023, Ulf Ryde (Sweden), *Recent development in quantum refinement of protein structures*
- 14th December 2023, Anna Krawczuk (Germany), *Dipolar group polarizability as a multipurpose tool for predicting molecular and bulk properties*
- 14th December 2023, Krzysztof Szalewicz (USA), *Reliable predictions of crystal structures entirely from quantum mechanics*
- 25th January 2024, Marek Żukowski (Poland), *Einstein-Podolsky-Rosen paradox, Bell's theorem, entanglement, GHZ paradox, 'nonlinear' crystals, quantum teleportation, and Nobel Prize 2022*
- 29th February 2024, Julia Contreras-Garcia (France), *Constructing new models to predict superconductivity from the electron density and localization*
- 29th February 2024, Eva Zurek (USA), *Theoretical design of light-element superconductors*

Financial support from ECA to schools, workshops, and congresses

In 2023 ECA was able to support 6 schools/workshops, 2 meetings, 1 open lab and the ECS8 with a total amount of € 10,250. This support is a key priority of the association to secure the dissemination of our field of research. The following list illustrates the details of different events:

European Crystallographic School

- 8th European Crystallographic School (ECS8), 18th to 24th June 2023 in Berlin, Germany

Other Meetings and Schools

- 19th BCA/CCG Intensive Teaching School in X-ray Structure Analysis, 25th March to 2nd April 2023 in Durham, UK
- Hot Topics in Contemporary Crystallography 5 – HTCC5 workshop, 16th April to 21th April 2023 in Dubrovnik, Croatia
- 1st Masuku Openlab, 16th to 26th May 2023 in Franceville, Gabon
- 8th International School on Biological Crystallization (ISBC2023), 21st to 26th May 2023 in Granada, Spain
- "Summer School on Mathematical Crystallography, 12th to 16th June 2023 in Nancy, France
- Third International School on Porous Materials - MOFsSchool2023, 19th to 23rd June 2023 in Come Italy
- 55th Course of the International School of Crystallography, 29th to 24th June 2023 in Erice, Italy
- International Conference on Crystal Growth and Epitaxy, ICCGE-20, 30th July to 4th August 2023 in Naples, Italy
- 11th International Conference of Hellenic Crystallographic Association (HeCrA) 20th to 22nd October 2023 in Larisse, Greece

Outlook

The first important ECA event will be the next European Crystallographic School in Nancy, France (24-30 June, 2024). Later that summer, the European crystallography community will gather in Padova, Italy, from 26th-31th August 2024. ECM34 will be immediately followed at the same venue by EPDIC18, the 18th European Powder Diffraction Conference. Elections for a new Executive Committee will take place at the Council Meeting in Padova.