# International Union of Crystallography

# Activities' Report - Year 2024

## Representative Delegate: Dr. Cinzia Giannini; Alternate Delegate: Dr. Edmondo Gilioli

### 1. Introduction

Crystallography is the scientific discipline that studies the atomic and molecular arrangement of solid matter, providing essential tools for understanding the chemical and physical properties of materials. Since Max von Laue's discovery of X-ray diffraction in 1912 and William Henry and William Lawrence Bragg's development of the structural analysis method, crystallography has revolutionized modern science, with applications in chemistry, physics, geology, biology, materials science, and even pharmaceutical technology. Worldwide, it remains a key discipline for the development of new drugs, advanced materials, and innovative technologies. Italy boasts a long tradition in crystallography, with scientists who have made significant contributions to the field. Notable among them are Giacomo Luigi Ciamician, who in the early twentieth century anticipated the study of molecular interactions with light. Today, numerous Italian institutions—such as the National Research Council (CNR), the Italian Institute of Technology (IIT), and various universities—host cutting-edge crystallography laboratories. Facilities like the European Synchrotron Radiation Facility (ESRF) and the European XFEL enable Italian researchers to collaborate internationally to study materials' structural properties at unprecedented resolutions. The Italian Crystallographic Association (AIC) promotes the discipline's development both nationally and internationally, facilitating collaboration between academic institutions and industry. Organizations such as the International Union of Crystallography (IUCr) foster research and international cooperation, supporting projects around the globe. One of the most important areas is structural biology, where crystallography has made it possible to elucidate the structures of key biomolecules—such as DNA (thanks to Rosalind Franklin, James Watson, and Francis Crick)—and numerous proteins essential to human health. These discoveries now enable the design of tailor-made drugs to treat diseases like cancer and viral infections. Crystallography is also crucial to developing new materials for electronics, energy, and nanotechnology. For example, understanding semiconductors' crystal structures has driven advances in microelectronics and optoelectronics. In Italy and worldwide, progress in this field will continue to shape research and technological innovation.

### 2. Main activities carried on by IUCr during 2023 relevant for Italy and for CNR

In 2024, Italy hosted major international events in the fields of crystallography and structural biology (see details in § 3). In Padua, the 34th European Crystallography Meeting (ECM34, 16–30 August) took place, featuring a rich program of lectures, microsymposia, and industrial exhibitions. As one of ECM34's satellite events, the Italian Crystallographic Association organized a School of Electron Crystallography. Also in Padua, the European Powder Diffraction Conference (EPDIC18, 30 August – 2 September) was held—the European conference dedicated to powder diffraction, with a focus on materials science, computational methods, and artificial intelligence. In Bari, AIC2024 In-Silico Structural Biology (28–31 October) convened—an intensive course on computational techniques for protein studies, combining theory and hands-on practice. Finally, the Italian Society for Synchrotron Light Conference (SILS 2024, 5–7 September) was hosted at the University of Calabria, bringing together experts in synchrotron radiation and free-electron lasers. During the event, participants toured the new STAR (Southern Europe Thomson Back-Scattering Source for Applied Research) facility—a symbol of Italian scientific innovation.

**3. Activities carried on by (Italian Delegate name) within the Union during 2024 and impact on the Italian scientific community**

In detail, it is important to highlight that Italy hosted the following international events:

- **The 34th European Crystallography Meeting (ECM 34, https://www.ecm34.org/)**, organized in Padua, Italy, from 26 to 30 August 2024 by the European Crystallographic Association (ECA). The conference program was particularly stimulating, featuring scientific presentations, meetings, special events, and a large industrial exhibition. The event included 3 plenary lectures, 14 keynote talks, and 42 microsymposia, covering the full spectrum of crystallographic topics. **ECM 34 Chairs:** Gilberto Artioli (member of the CNR–IUCr Commission) and Giuseppe Zanotti.
- **The European Powder Diffraction Conference (EPDIC18, https://cristallografia.org/blog/2024/07/04/epdic18-updates/)**, the only conference in Europe entirely dedicated to all aspects of polycrystalline materials analysis by diffraction methods. It brought together experts from universities, research institutes, and instrument manufacturers to share their knowledge and discuss current trends and challenges in powder diffraction. EPDIC18 was a lively three-day scientific conference, offering numerous learning opportunities on all aspects of powder crystallography, alongside a major commercial exhibition. The scientific program covered the latest advances in crystallography and related sciences, spanning materials science, computational methods, artificial intelligence, and scientific instrumentation. **EPDIC18 Chairs:** Rosanna Rizzi and Annamaria Mazzone.
- **AIC2024 In-Silico Structural Biology (28–31 October 2024, Bari, Italy; https://www.gene2structure.it/issb-programme/)**. This course provided a comprehensive overview of in-silico methods for predicting and studying protein structures and properties. Theoretical sessions equipped participants with a solid grounding in the fundamentals of computational modeling, including key concepts in molecular dynamics and AI techniques applied to structural biology. The course also featured modules on molecular docking for ligand–protein interaction analysis and on molecular dynamics driven by experimental structural data. In addition to lectures, practical sessions enriched the learning experience by allowing participants to apply their new knowledge directly—through guided simulations and modeling activities, they experimented with advanced tools and software, honing their skills in protein-structure analysis and manipulation.
- **ElCryS 24: Electron Crystallography School 2024 (24–26 August 2024, Padua, Italy; https://elcrys24.sciencesconf.org/?lang=en)**. Organized as a satellite event of ECM 34 by the International Union of Crystallography (IUCr), the IUCr Commission on Electron Crystallography, ECA's SIG4, and the Italian Crystallographic Association (AIC), this school reflected the growing interest in electron diffraction over the past decade—driven by automated data collection on transmission electron microscopes. Three-dimensional electron diffraction enables analysis of single crystals only a few tens of nanometers in size. This technique is effective for determining new organic and inorganic structures, studying light atoms, ionic charges, and chiral structures. Ten European experts delivered theoretical and practical lectures, and students followed a complete data-processing workflow, interacting directly with electronic-crystallography software developers—thereby fostering innovation and scientific collaboration.
- **2024 Annual Conference of the Italian Society for Synchrotron Light (SILS 2024, 5–7 September 2024)**, held at the University of Calabria in Rende (CS). Aimed at fostering interaction among Italian researchers in synchrotron radiation, free-electron lasers (FELs), and advanced light sources in general, it provided an opportunity to present the latest scientific results across various research fields and to assess the state of the art and future prospects of light-source technologies (https://sites.google.com/view/sils2024/home). **Member of the Scientific Committee:** Cinzia Giannini. During the event, participants visited the new STAR (Southern Europe Thomson Back-Scattering Source for Applied Research) research facility.

**4. Evaluation of the participation in terms of benefits and membership cost**

The annual IUCr membership fee paid by the CNR (6,000 Swiss francs) is justified by the substantial benefits it brings—not only to the national crystallographic community but also to numerous related scientific fields that make extensive use of crystallographic techniques and applications. Moreover, from an economic-return perspective, it is important to note that the majority of international crystallography events organized in Italy receive financial support from the IUCr, thereby contributing to the growth of the field in our country.

## 5. Evaluation of Italians' attendance and how to improve interest and involvement

To broaden the interest and engagement of the Italian scientific community in IUCr activities, the following strategies can be adopted:

- **Enhanced outreach:** Intensify awareness-raising and informational activities about crystallography, highlighting its applications and the importance of Italy's participation in international initiatives.
- **Collaborative research projects:** Promote and facilitate collaborations between Italian crystallographers and international researchers, encouraging synergies that can lead to significant innovations in the field.
- **Engagement of young scientists:** Develop initiatives aimed at students and early-career researchers, offering training opportunities, mentorship, and participation in international conferences and scientific programs.
- **Diversification of research areas:** Expand the scope of crystallography by fostering interdisciplinary collaborations with other scientific domains. This approach would encourage broader integration of crystallographic methods across diverse research fields.
- **Strengthening communication:** Improve channels of communication between the CNR–IUCr Commission and the Italian crystallographic community through regular newsletters, webinars, and online forums, ensuring more effective information dissemination and dialogue.
- **Greater Italian representation within the IUCr:** Bolster the presence of Italian experts in IUCr decision-making bodies—such as the Executive Committee, Commissions, and editorial boards of scientific journals.
- **Scientific publications:** Encourage Italian researchers to publish their studies in IUCr journals, thereby increasing the visibility and impact of Italian research on the international stage.

Implementing these strategies would consolidate the relationship between the Italian crystallographic community and the IUCr, fostering greater participation, collaboration, and global visibility.

## 6. Italian experts with important roles within the IUCr or within related Commissions and Programs (if known)

Within the IUCr Commissions and Journals, Italy holds various roles:
- 11 IUCr Commission members
- 15 IUCr Commission advisors
- Angela Altomare (IC–CNR Bari) serves as "Section Editor" of Acta Crystallographica A
- Chiara Massera (University of Parma) serves as "Section Editor" of Acta Crystallographica E
- Cinzia Giannini is a member of the International Program Committee for the Twenty-Seventh Congress of the International Union of Crystallography (11–18 August 2026, Calgary, Canada)
- 3 Co-Editors
- 4 peer-review committee members

## 7. Short summary about the 2024 CNR Commission activities

CNR benefits from the insights and advice of the "Commission for CNR's Participation in the IUCr." The Commission includes Angela Altomare, Gilberto Artioli, Cecilia Lalle (Secretary), G. Diego Gatta, Cinzia Giannini (Chair), Edmondo Gilioli (Scientific Secretary), Andrea Ienco, Andrea Ilari, Chiara Massera, Marzio Rancan, and Michele Saviano.

The CNR–IUCr Commission plays a key role in coordinating Italy's participation in the International Union of Crystallography (IUCr). Composed of Italian experts in the field—drawn from both research institutions and academia—the Commission serves as Italy's "National Committee," as provided for in the IUCr Statutes. This role brings numerous advantages, including:

- Acting as link between Italian crystallographic community and IUCr.
- Providing guidelines and recommendations to ensure Italy's effective involvement in IUCr activities.
- Supporting CNR in international initiatives and projects promoted by IUCr.
- Reviewing and offering opinions on proposed amendments to IUCr regulations.
- Nominating candidates for elective IUCr offices, including President, the Executive Committee, and Commissions.
- Proposing plenary and keynote speakers for the IUCr Congress, as well as themes and chairs for scientific sessions.

- Strengthening IUCr education, outreach, and training activities in countries where crystallography is less developed—such as parts of Africa, Albania, and Montenegro—by promoting the creation of shared laboratories.
- Showcasing the expertise and work of Italian researchers internationally through participation in IUCr initiatives.

In 2024, several Commission members took part in courses and events (including giving talks) and contributed to organizing conferences.

**8. Notes (if any)**

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**9. Conclusions**

Over the 2024, numerous initiatives in Italy have demonstrated the ongoing commitment to promoting and developing crystallography both nationally and internationally. Among the most prominent events were the 34th European Crystallography Meeting (ECM34, Padua, 16–30 August), the European Powder Diffraction Conference (EPDIC18, Padua, 30 August–2 September), the In-Silico Structural Biology Congress (AIC2024, Bari, 28–31 October), and the Italian Society for Synchrotron Light Conference (SILS 2024, Rende (CS), 5–7 September).

The CNR–IUCr Commission continues to play a crucial role in coordinating national activities within the IUCr. Many of its members hold prominent positions within IUCr governance, Commissions, and journals.

However, it remains essential to strengthen the interest and participation of the Italian scientific community in IUCr activities. Suggested initiatives include enhanced outreach, the promotion of collaborative research projects, incentives for young scientists' involvement, expansion of research areas, and the enhancement of communication channels—with particular attention to social media. From a scientific standpoint, publishing studies in prestigious international journals remains of primary importance.

Italy has also made significant contributions to the new frontiers of crystallography, going beyond the classical definition of a crystal. The adoption of advanced technologies—such as synchrotrons and free-electron lasers—has greatly expanded research prospects, paving the way for more innovative studies and applications across various fields.

The Italian crystallographic community is also involved in organizing activities in Africa, including research and educational collaborations with several African countries.

In conclusion, Italian participation in the IUCr in 2024 confirms a sustained commitment to advancing crystallography, making a valuable contribution to the international scientific community and to the challenges of the future.

Signature

Place and date

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