

# International Union of Crystallography

## Activities' Report - Year 2023

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### 1. Introduction

*"We are like dwarfs standing on the shoulders of giants,"* said Bernard of Chartres. We can see more than the giants and see even further because we are lifted and carried high by their immense stature.

Crystallography has encountered many of these giants. William Henry Bragg and William Lawrence Bragg, British physicists and crystallographers, father and son, are two of the most well-known. Additionally, women of exceptional scientific value, such as Dorothy Hodgkin, the discoverer of the structure of penicillin, or Rosalind Franklin, who gathered magnificent X-ray diffraction data on DNA (the famous Photo 51), have made significant contributions.

At least 30 Nobel Prizes have been awarded for work directly or indirectly related to crystallographic studies. It is noteworthy that such studies have been fundamental in various disciplines (physics, chemistry, mineralogy, medicine) because Crystallography is an intrinsically versatile discipline. It has been essential for structural analysis over the past hundred years, maintaining a prominent role to this day. Crystallography has allowed us to "observe" the world atom by atom, providing three-dimensional information about electron density and revealing structural mechanisms influencing specific functions in new materials and biological molecules. Crystallography has become indispensable, playing a crucial and relevant role in various production sectors, from the pharmaceutical and agri-food industries to cultural heritage preservation, to name a few examples.

Crystallography was considered useful only in the presence of a material with a long-range three-dimensional translational periodicity. This was its only field of application until 1970. In that year, X-rays were generated by a synchrotron at the National Research Center for Nuclear Physics (DESY) in Hamburg. With synchrotrons and, even more so, with the first operation of the Free Electron Laser (FEL) for X-rays in 2009 at the SLAC National Accelerator Laboratory in California, scientists began working with coherent X-rays. This allowed access to the local structure of non-periodic objects. The advent of FELs with inherently coherent X-rays, producing pulses lasting a few femtoseconds ( $1 \text{ fs} = 10^{-15} \text{ s}$ ), three orders of magnitude shorter than those from synchrotrons, has been revolutionary. This temporal precision enables real-time observation of biological, chemical, and physical processes occurring on the femtosecond scale. Modern instruments allow for the collection of petabytes ( $10^{15}$  bytes) of data per day for a single experiment, requiring significant infrastructure for data collection and analysis, as well as investments in artificial intelligence.

This brief overview illustrates how the methodological, experimental and computational frontiers of Crystallography have greatly expanded, especially in the last two decades, also beyond the confines of a discipline that studies only crystals (according to the traditional definition of a crystal), representing a research area at the intersection of various disciplines—a fertile ground for the development of new ideas, high-impact technologies, and a unique environment for cutting-edge scientific research.

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

In 2023, a significant crystallographic event for Italy and the international crystallographic community was the Twenty-Sixth Congress and General Assembly of the International Union of Crystallography, held from August 22 to 29 in Melbourne, Australia (<https://iucr2023.org/>). Despite considerable expenses and the distant location of the Twenty-Sixth IUCr Congress, Italy actively participated. Recommendations put forth by the CNR-IUCr Commission to the IUCr, suggesting the roles of Italian scientists at the Congress and within Commissions and Journals, were well-received.

Italian involvement at the Twenty-Sixth IUCr Congress included:

- 3 members on the International Program Committee
- 1 keynote speaker

- 11 speakers
- 9 chairs of Microsymposia

During the Congress, the General Assembly of the Union played a crucial role, renewing governing bodies such as the Executive Committee, Commission and Editorial Board members. Italian delegates Analisa Guerri (Università di Firenze), Gilberto Artioli (Università di Padova), Dritan Siliqi (IC-CNR Bari) participated in the IUCr General Assembly. Angela Altomare (IC-CNR, Bari) was confirmed as a member of the Executive Committee for the next three years.

### **3. Activities carried on by (Italian Delegate name) within the Union during 2022 and impact on the Italian scientific community**

It is noteworthy that Italy hosted the following international events:

- International Conference on Crystal Growth and Epitaxy-ICCGE-20, 30 July-4 August 2023, Naples, Italy (<https://www.iccge20.org/>). The scientific program was organized on the following topics: 2D Materials; Advances in observation and characterization methods; Bulk crystal growth; Composite and hybrid crystals; Crystalline solids for drugs and pharmaceuticals; Crystallization of organic and biological systems; Crystals for photovoltaics and green energy; Functional crystals; Fundamentals of nucleation and crystal growth; Growth at the nanoscale: nanocrystals, nanowires, nanomaterials; Industrial crystal growth technology and equipment; Modelling and artificial intelligence of crystal growth processes; New methods and techniques for crystal growth; Optical crystals; Semiconductors; Structural defects and impurities in crystalline materials; Surfaces and Interfaces; Thin films and epitaxial growth; Topological quantum materials
- 18th International Summer School on Crystal Growth-ISSCG-18, July 23-28 2023, July 23-28 2023, Parma, Italy (<https://isscg-18.unipr.it/index.php>), co-organized by the University of Parma and the CNR-IMEM (Institute of Materials for Electronics and Magnetism) in Parma, in July 23-28, 2023. The school is co-chaired by Roberto Fornari (Università di Parma) and Edmondo Gilioli (CNR-IMEM) and promoted and sponsored by the IOCG - International Organization for Crystal Growth (two IOCG grants student from Brazil and from Poland) and the AIC - Italian Crystallographic Association (one grant for young researchers affiliated to AIC). The ISSCG-18 programme included 15 lecturers, (29 hours in total) on fundamentals, technology & processes and specific case studies, focusing on: theoretical and experimental aspects of crystal growth of different types of crystalline materials: thermodynamic and kinetic fundamentals; modelling and simulation; surfaces and interfaces; polymorphism; growth technologies for single crystals; epitaxy and thin films; nanocrystals and 2D crystals; biological crystallization; defects in crystalline materials; case studies of technologically-important materials.
- AIC2023 International School 'Electron Crystallography A deep dive into nanocrystals', 3-6th July 2023, Pisa, Italy (<https://school2023.cristallografia.org/>). Students have been first introduced to the peculiarities of ED and then driven through data acquisition procedures and data reduction software. The school covered both well-established 3DED protocols, based on step-wise acquisition and beam-precession, and more recent protocols based on continuous data acquisition through latest fast and sensitive detectors, particularly suitable for organics and macromolecules. Methods and routines for structure solution and refinement were described, with a special focus on the treatment and use of residual dynamical effects. Specific features and issues related with inorganic, small-molecule organics and macromolecular compounds were stressed, with first-hand several softwares for 3DED data reduction, structure solution and structure refinement. Cutting-edge methodologies, like serial-ED, phase-orientation mapping and electron pair-distribution function (ePDF) were also introduced.

Italian scientific activity has involved the organization also of national events:

- The 50th Italian Crystallographic Association Congress was held in Bologna, 5-8 September 2023 (<https://eventi.unibo.it/aic-meeting-2023>). Michele Zema (University of Bari), IUCr outreach, was invited as a plenary speaker, and illustrated many of initiatives supported by the IUCr aimed at increasing awareness of crystallography in all parts of the world, showcasing its fundamental role across various scientific disciplines, and emphasizing its contribution to the general public and the younger generation.
- The Italian Synchrotron Radiation Society (SILS) Annual Conference 2023 held in Rome at the Sapienza University from Wednesday 30 August until Friday 1 September 2023. The SILS Annual Conference is committed to continuing the tradition and fostering interaction among the Italian researchers working in the field of synchrotron radiation, free electron lasers and sources of electromagnetic radiation, in a crystallographic framework. It serves as a forum to highlight recent scientific results in different fields and to present the current status and future directions of synchrotron radiation and free electron laser sources. The programme featured: plenary lectures delivered by highly recognized international experts in different fields; plenary session to update on the status and future upgrades of synchrotron and FEL facilities; a set of thematic

micro-symposia; an open session and a Young Investigator session; a poster session (<https://www.ba.ic.cnr.it/sils2023/>).

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

The Commission ensures the coordination of the Italian participation in IUCr and is indeed composed of Italian experts of crystallography from the research and academic world. The Commission fulfills the role of the Italian "National Committee" as stipulated by the IUCr Statute. Therefore, the benefits derived from the following items:

- it serves as a liaison between the Italian community and the IUCr,
- it provides guidance and proposals for effective Italian participation in IUCr activities.
- it offers necessary support to CNR on matters related to initiatives and international activities promoted by IUCr.
- it provides opinions on proposed changes to IUCr regulations.
- it put forth proposals for nominations to all elective bodies of IUCr (President, Executive Committee, Chairs, and members of Commissions).
- it makes suggestions for plenary and keynote speakers for the IUCr congress and for scientific session themes and chairs.
- it enhances IUCr activities related to education, outreach, and training in specific countries where crystallographic culture is less prevalent (in Africa, Albania, and Montenegro) to establish shared laboratories.
- it promotes, through Italian participation in IUCr activities, the activities and expertise of Italian researchers at the international level.

The cost incurred by CNR for membership (the membership fee for IUCr has been CHF 6,000.00) seems sustainable in light of the significant benefits for both our national crystallographic community and for many adjacent scientific sectors that extensively utilize crystallographic techniques and their applications. From an economic return perspective, it should also be emphasized that almost all crystallography events organized in Italy receive some financial support from the Union

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

To further enhance the interest and involvement of the Italian scientific community in the IUCr, the following proposals can be considered:

- **Increased Outreach:** Strengthen efforts in outreach programs to educate and create awareness about crystallography, its applications, and the importance of participation in international initiatives.
- **Collaborative Research Projects:** Encourage and facilitate collaborative research projects between Italian crystallographers and their international counterparts. Foster partnerships that can contribute to cutting-edge advancements in the field.
- **Youth Engagement:** Implement initiatives targeting young researchers and students, providing opportunities for skill development, mentorship, and active participation in international conferences and programs.
- **Diversification of Research Areas:** Promote the diversification of research areas within crystallography, encouraging interdisciplinary collaborations. This can attract researchers from different scientific disciplines, fostering a broader and more inclusive community.
- **Communication Channels:** Enhance communication channels between the CNR-IUCr Commission and the Italian crystallographic community. Regular newsletters, webinars, and forums can facilitate transparent information sharing and discussions.
- **Active response to IUCr requests:** Increasing Italian representation within the Union's bodies (Executive Committee, Commissions, Journals).
- **Scientific publications:** Encouraging the Italian crystallographic community to publish in IUCr Journals.

By implementing these proposals, there is potential to strengthen the bonds between the Italian crystallographic community and the IUCr, fostering increased interest, participation, and collaboration on a global scale.

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

Within the IUCr Commissions and Journals, Italy held various roles:

- 11 members of IUCr Commissions
- 15 consultants of IUCr Commissions
- Angela Altomare (IC-CNR Bari) serves as a "Section Editor" of Acta Crystallographica A and has been confirmed as a member of the Executive Committee for the next three years.
- Chiara Massera (Parma University) holds the position of a "Section Editor" of Acta Crystallographica E
- 3 Co-Editors
- 4 review board members
- Michele Zema (University of Bari) served as the IUCr outreach officer.

## 7. Short summary about the 2023 CNR Commission activities

The CNR benefits from the insights and advices of the "Commission for the Participation of the CNR in the IUCr." This commission, renewed in 2023, comprises Angela Altomare, Gilberto Artioli, Virginia Coda Nunziante, Cecilia Lalle, G. Diego Gatta, Cinzia Giannini (President), Edmondo Gilioli (Scientific Secretary), Andrea Ienco, Andrea Ilari, Chiara Massera, Marzio Rancan, Michele Saviano.

On July 13, 2023, at 3:00 PM, the Commission gathered through online mode. After a short presentation of the attendees, the main discussion was about the contribution of the Italian community to the XXVI IUCr Congress.

## 8. Notes (if any)

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## 9. Conclusions

In conclusion, the Italian participation in the International Union of Crystallography (IUCr) in 2023 has demonstrated an active and significant involvement in the international crystallographic community. The 26th Congress and General Assembly of the IUCr in Melbourne marked a crucial moment, with the presence of numerous Italian members in various roles, confirming the importance and relevance of Italian crystallography on the global scientific stage.

Activities conducted in Italy in 2023 included international conferences, summer schools, and national congresses, showcasing a consistent commitment to promote and develop crystallography at both local and international levels. Participation in events like the International Conference on Crystal Growth and Epitaxy (ICCGE-20) in Naples, the International Summer School on Crystal Growth-ISSCG-18 in Parma and the International School on Electron Crystallography in Pisa further solidified Italy's presence in the crystallographic scientific landscape.

The CNR-IUCr Commission played a fundamental role in coordinating Italian participation in the IUCr, acting as a bridge between the Italian community and the Union. Its members contributed in various ways, actively participating in the IUCr Congress and taking on prominent roles within the IUCr governance, Commissions and Journals.

To further enhance the interest and involvement of the Italian community in the IUCr, several initiatives are proposed, including increased outreach, collaborative research projects, engagement of young researchers, diversification of research areas, and enhancement of communication channels, active response to IUCr requests, scientific publications.

Lastly, Italy has made a significant impact on the new frontiers of crystallography, surpassing the traditional definition of a crystal. The introduction of technologies such as synchrotrons and X-ray free-electron lasers has greatly expanded the possibilities of study, paving the way for advanced research and innovative applications in various fields.

Overall, Italian participation in the IUCr in 2023 reflects a consistent commitment to promote crystallography, contributing significantly to international science and addressing the new scientific challenges of the future.

Signature

Place and date