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President's Letter – Winter 2024

Santiago García-Granda

As we bid farewell to the year 2024 and look forward to the beginning of 2025, I write this brief note for the winter Newsletter of the IUCr with best wishes to the people who make up this scientific family.

2024 has been a busy year in terms of scientific meetings of our regional associations, all of them very successful, the last and most recent being the Asian Crystallographic Association (AsCA) meeting in Kuala Lumpur, Malaysia. The regional impact of the IUCr is one of the most effective ways to bring the IUCr closer to the scientific societies related to structural science. Once again we have witnessed the awarding of a Nobel Prize directly related to structural science and macromolecular crystallography. Our community has produced some very creative videos with ingenious ideas for the crystallization competitions that are held in many countries. The new EC Outreach Committee is overseeing support for proposed outreach initiatives around the world. We have also boosted the prominence and leadership of women scientists in our community resulting in an impact on global science.

The reorganization of staff in our Chester office is being completed successfully, both in the editorial, administrative and outreach sections, with Kezia Bowman now looking after the IUCr Newsletter and the addition of Harriet Jackson in the office. There are great expectations for an increase in our editorial strength with the addition of the new Head of Publishing Strategy, who is expected to join the Chester editorial team in the new year.

The Executive Committee met virtually on 12 November, and the Finance Committee will meet virtually on 18 December. The Finance Committee will meet in person in Lund, Sweden, on 24-25 March 2025, just after the annual meeting of the Journals Management Board which will take place in Chester on 20-21 March. It is a priority for the Executive Committee to return the activity levels of our journals to those in 2019 and to recover their capacity to produce the resources to cover the funding of our projects, especially the support to young scientists and the promotion of structural science in less developed geographical areas. In this endeavor, it is also important that the Finance Committee is able to identify the most productive and secure investments for the future of our financial health.

2025 will be a year of consolidation of the organization of the Congress and the 27th General Assembly in Calgary, Canada. As with every congress, the participation and support of our commercial partners will be very important in order to be able to organise a commercial exhibition as attractive as our scientific congress. It is important that no participation is hampered by bureaucratic or other issues, and we will strive to facilitate the widest possible participation and, in particular, to promote the presence and influence of younger researchers.

All IUCr Commissions are proposing members of the International Programme Committee (IPC) and selecting the more attractive speakers for the Plenary and Keynote Lectures, as well as the most appealing Microsymposia, showing the impact of crystallography and structural science in solving the challenges of the present and future of our planet.

The International Science Council (ISC) Elections for the shortlist of candidates for renewal of the ISC Governing Board will take place in Oman, in the framework of the Muscat Global Knowledge Dialogue and Third ISC General Assembly, in January 2025. The IUCr will be represented by our Vice-President Professor Graciela Díaz de Delgado.

Following its inaugural meeting, the IUCr Early Career Scientist Division (ECSD) met on 18 November 2024, and several decisions were taken to develop this important division of IUCr. The first elected Chair and Co-chair were Rebecca Clulow (ECA) and Orbett Alexander (AfCA). Kara Zielinski (ACA) was nominated as a member of the Division to serve on the International Program Committee (IPC). Actions were planned to

increase the visibility of the new IUCr Division in the existing communities and to organize meetings for young scientists in the field of structural sciences. All of the initial group are actively producing new ideas and developing the framework and networks to have a major impact on the present and the future of IUCr.

As usual, I end this letter with deep gratitude to all those who form and make our organisation work, the Regional Associates, the IUCr Commissions and Committees, Editors, Co-editors, referees and authors of our journals, our Chester staff and all individual structural scientists, women and men.

Thanks to IUCr Newsletter Editor Mike Glazer, and his team, and thanks to all contributors for making possible, as with every issue, a new issue that continues to be the reference communication for our community.

Thank you all for helping to keep the momentum of the IUCr going, wherever you are in the world.

Enjoy the holiday season with your families, colleagues and friends!

Best wishes for the best personal and professional development in 2025.

Editorial

Mike Glazer

I recently attended a meeting of the Biographical Memoirs Committee of the Royal Society where a discussion was had about how to promote the Memoirs to the wider public. I was reminded that some time ago, we ran an article (https://www.iucr.org/news/newsletter/volume-28/number-1/royal-society-ibiographical-memoirsi-now-free-to-read-online!) on the memoirs of crystallographers who were Fellows of the Royal Society. When one considers the great successes of crystallographers since the initial work of Laue in Germany and the Braggs, father and son, in England in 1912, together with the extraordinary number of Nobel Prizes awarded for research in or related to crystallography (roughly 30), it is not surprising to find so many biographical memoirs of crystallographers in the Royal Society archives. So, for those of you who missed the earlier article, I thought it would be worth recalling that there is a wealth of interesting material available on the Royal Society website. Since that list was published in the Newsletter, we have to add the memoirs of Michael Woolfson, who died in 1919 (https://royalsocietypublishing.org/doi/10.1098/rsbm.2021.0018), and Louise Johnson, who died in 2012 (https://royalsocietypublishing.org/doi/10.1098/rsbm.2021.0038).

It is not often that a particular science suddenly has most of its basic tenets overthrown, but that is exactly what occurred 40 years ago in Crystallography. I recall how surprised (shocked?) I was to hear then that some crystals had been discovered that completely overturned the received dogma on the nature of symmetry in crystals. Like most crystallographers, I had been brought up in the belief that crystals could not have 5-fold rotational symmetry and that according to the so-called Crystallographic Restriction Theorem, only 1 (i.e. no symmetry),2,3,4 and 6-fold symmetry was allowed. Dan Schechtman's discovery and subsequent Nobel Prize (2011) made crystallographers rethink what they thought they knew about crystal symmetry. In this issue of the Newsletter, Istvan Hargittai has written an article for us (ref), recording some aspects of that discovery and how it came to be in collaboration with others at the time. Today, the existence of the so-called quasicrystals is completely accepted, and numerous papers and books have been written on this subject. To be true, this is mainly of an academic nature since quasicrystals have yet to find much application, and the Restriction Theorem still applies to most crystals that we study. Quasicrystals belong to a class of crystals known in general as aperiodic crystals, where the usual concept of periodicity (i.e., repetition of atoms or molecules to define what we call the crystal structure) breaks down in three dimensions. However, when one considers periodicity occurring in a higher dimension (mathematicians have no problem with this!), typically in a 6-dimensional space, quasicrystals then become understandable as a projection down onto our 3-dimensional world. So, when we think of what a crystal means, we have to revise previously held views. See, for example, https://www.iucr.org/news/newsletter/etc/articles?issue=151351&result_138339_result_page=17. It is interesting to note that some clever scientists, such as Roger Penrose and, especially, the crystallographer Alan Mackay at Birkbeck College London, had already been playing around with these ideas long before the discovery of quasicrystals. I recall, as a young PhD student, attending lectures by Alan, who taught us how to draw different crystal shapes, and he introduced some rather unusual thoughts on crystal symmetry, but I have to admit that I did not appreciate his ideas at the time!

Oxford

JAPAN-TAIWAN BILATERAL SEMINAR ON CRYSTALLOGRAPHY: "FRONTIER OF CRYSTALLOGRAPHY"

Hiroyoshi Matsumura and Kazuya Hasegawa

In November 2024, the Institute for Protein Research (IPR), the Research Center for Crystalline Materials Engineering (RCCME), and the Comprehensive Research Organization for Science and Society (CROSS) successfully hosted the Japan-Taiwan Bilateral Seminar on Crystallography: "Frontiers of Crystallography." The event was held at the FUJI Hall, located in the EI (Emergent/Innovative) Engineering Building at Nagoya University, and brought together around 30 participants from Japan and Taiwan.

The Japan-Taiwan Bilateral Seminar on Crystallography, originally established in 1990, was temporarily suspended due to the COVID-19 pandemic but has now resumed. With the goal of advancing crystallography in both Japan and Taiwan and fostering ongoing personal connections, leading researchers were invited to engage in research exchanges.

In the opening remarks, Prof. Kurisu from Osaka University and Prof. Nei-Li Chan from National Taiwan University, who have maintained a close relationship over 20 years, provided their experience on the bilateral relationship. Prof. Hasegawa from Nagoya University introduced RCCME, highlighting the structural science conducted at the center. The scientific session featured high-level presentations by eight young researchers in fields such as structural biology, MicroED, and functional small molecules, as outlined below.

Naruhiko Adachi, Japan "Setup and operation of 3DED/microED experiments at KEK and Tsukuba Univ."

Yu-Yuan Hsiao, Taiwan "Structural analysis of TREX1: From catalytic property identification to inhibitor development"

Kazuki Kawahara, Japan "Structural biology of the type IV pillus from enteric bacterial pathogens"

Shih-Ming Lin, Taiwan "Calcium-dependent modulation and lectin domain function in the activation of Vibrio campbellii α-hemolysin"

Toshiyuki Sasaki, Japan "Tailoring structural analysis of functional small-molecule crystals with X-ray and electron diffraction methods depending on crystal properties"

Chyuan-Chuan Wu, Taiwan "Structural basis of mitochondrial DNA degradation machinery"

Yuya Hanazono, Japan "Structural analysis of amide protons using high-resolution neutron crystallography"

Wen-Ting Lo, Taiwan "Structural basis of class II phosphoinositide 3-kinase regulation and pharmacological inhibition"

At the end of the scientific session, Prof. Nakagawa from Osaka University provided an overview of the upcoming AsCA 2025 conference, which will be held in Taipei next year and co-organized by Japan and Taiwan. In his closing remarks, Prof. Sugiyama, President of CrSJ, highlighted the longstanding bilateral relationship in crystallography and underscored the importance of continued collaboration. Following the symposium, a banquet was held in Nagoya University's cafeteria, where participants enjoyed lively discussions over beer and wine. This meeting showcased the strong ties built over three decades, with knowledge and camaraderie passed from generation to generation. We believe this symposium will contribute to the success of AsCA 2025.

Eleventh Polish Crystal Growing Competition for Schools 2024

Monika Oboz, Magdalena Szubka

The first edition of the Polish Crystal Growing Competition for Schools organized at the Institute of Physics of the University of Silesia in 2014 was inspired by Dr. Hanna Dąbkowska, a member of the IUCr Commission for Crystal Growth. The competition immediately gained great popularity and, since 2014, has been held every year.

Over 220 participants from 45 different towns participated in this year's eleventh edition of the competition, sending over 300 good-quality crystals.

Traditionally, the jury selected three winners and distinguished over 20 works. The award ceremony occurred on June 13, 2024, during the "Crystals: order, beauty and utility" conference at the Institute of Physics of the University of Silesia in Katowice.

It was held under the patronage of the dean of the Faculty of Science and Technology, prof. Danuta Stróż and director of the Institute of Physics of the University of Silesia, prof. Sebastian Pawlus.
During the conference, lectures were given by invited outstanding specialists from national research centers, such as the Institute of High Pressures of the Polish Academy of Sciences (UNIPRESS) and the Institute of Molecular Physics of the Polish Academy of Sciences.

At the awards gala, there was a presentation of the winners and participants distinguished in the competition and an award ceremony.

The conference ended with a poster session of the winners and authors of distinguished works, during which awards for the best poster were presented.

The conference and the competition awards gala took place during Crystal Week, part of the celebrations organized by the Academic Consortium of seven public universities as part of the European City of Science 2024, a title awarded to Katowice by the European Commission.

The Polish Crystal Growth Society and the Crystallography Committee of the Polish Academy of Sciences provided the patronage of the competition.

The event was co-financed by the Silesian Voivodeship - Co-organizer of the European City of Science Katowice 2024.

The winners of the competition

Joanna Ajdukiewicz

Teacher Agata Bladoszewska

1st Bilingual Secondary School

named after Edward Dembowski

Gliwice

1st place

C6H8O7

Wiktor Januszkiewicz

Teacher Maria Rogozińska - Szymczak

XXXV General Secondary School with Bilingual Departments named after Bolesław Prus

Warszawa

2nd place

K(Al,Cr)(SO4)2 12H2O

Bruno Głogowski

Teacher Agnieszka Cacek

Primary School No. 221 with Integration Departments named after Barbara Bronisława Czarnowska

Warszawa

3rd place

KAl(SO4)2 x 12H2O

ACA2024 Meeting Recap

K. Stevens | October 25, 2024

The 2024 American Crystallographic Association (ACA) Annual Meeting was held from July 7-12, 2024, at the Denver Marriott Tech Center in Denver, Colorado. This gathering of structural science professionals, including researchers and industry experts, provided a vibrant platform for scientific exchange, networking, and exploring the latest advancements in crystallography. With attendance surpassing 600 and more than 400 oral and poster abstracts submitted, the growing relevance of structural science was incredibly evident. The meeting brought together seasoned scientists and early-career researchers who engaged in diverse sessions, workshops, and social events.

We are grateful to our members whose donations have supported the ACA student travel grant, and we extend our thanks to the IUCr for their generous grant, both of which enabled us to award over 30 travel grants to early-career scientists, allowing them to attend and actively participate at ACA2024.

From left to right above: Catherine Drennan presents her keynote address; attendees engage with virtual reality in the exhibit hall; workshop participants collaborate.

A highlight of the meeting was the keynote address by Catherine Drennan, a prominent chemist and biochemist, who captivated attendees with her talk, “Shake, Rattle, & Roll: Capturing Snapshots of Proteins in Action.” Known for her passion for "molecular storytelling," Dr. Drennan shared insights into her lab’s use of X-ray crystallography and electron microscopy to capture enzymes in action, offering a remarkable glimpse into the molecular “dances” that drive biochemical reactions.

Following the keynote, attendees gathered in the exhibit hall, where over 30 companies showcased products and services essential to structural science. Many of these exhibitors, including Thermo Fisher Scientific, Xenocs Inc., Rigaku Americas Corporation, DECTRIS Ltd, the American Institute of Physics, Bruker AXS, Quantum Detectors, Gatan, FEI Electron Optics BV (The Netherlands), Stoe Corporation, MiTeGen, SPT Labtech, Stoe Corporation, Crystal Growth & Design, Formulatrix, MiTeGen, the Hampton Research Corp., Xenocs Inc., Waters|Wyatt Technology, Anton Paar, NanoSoft, LLC and Altos Labs, among others, also supported the meeting as sponsors, helping to fund speaker travel and other essential expenses.

From left to right: The IUCr2026 booth distributing congress materials, the ACA Council in session, and a view of one of the session rooms.

The exhibit hall also featured a booth spotlighting the Twenty-Seventh Congress and General Assembly, to be held in Calgary, Alberta, Canada, from August 11-18, 2026. Hosted by the ACA, the Canadian National Committee for Crystallography (CNCC), and the US National Committee for Crystallography (USNC/Cr), the booth showcased exciting plans for the congress in Calgary's vibrant setting.

ACA2024 hosted over 30 sessions covering a number of diverse structural science topics and five highly attended workshops including Workshop 1: Advanced Structure Refinement with Olex2 & NoSpherA2, Workshop 2: Applications of Small Angle Scattering to Structural Biology: An Introduction, Workshop 3: Hands-on CryoEM Sample Preparation &Data Collection Workshop Using CryoEM Merit Badges, Workshop 4: Simple & Advanced Single Crystal X-Ray Structure Refinement Using ShelXle and Workshop 5: Crystallographic & Cryo-EM Structure Solution with Phenix.

The Young Scientist Interest Group (YSIG) played an active role in supporting early-career researchers, organizing a mixer and the popular Three Minute Thesis (3MT) competition. This competition challenged young scientists to present their research in three minutes. Manju Ojha from the University of Maryland, Baltimore County, claimed first place with her presentation, 'Structure of saguaro cactus virus 3′ translational enhancer mimics 5′ cap for eIF4E binding.' Nicholas Bragagnolo from York University earned second place for his talk, 'TraG-edy to Triumph: How Challenges in Crystallisation Efforts of TraG Led to Success.' In third place, Chhandosee Ganguly from the University of Oklahoma presented 'Simple Techniques to Improve Particle Distribution and Data Quality for Dynamic Protein-Nucleic Acid Complexes.

From left to right: Attendees board the bus after the YSIG mixer; poster presenters receive awards at the banquet; ACA President Allen Oliver addresses the audience.

Beyond the scheduled early career activities, the week was filled with engaging moments. Games unfolded spontaneously in the lobby, and one evening, an impromptu karaoke session infused a conference room with lively energy. In a touching instance of mentorship, a young attendee, sits captivated in the speaker-ready room as a seasoned presenter Larry Andrews rehearsed his slides. The young attendee stayed, drawn into Larry's presentation, as he graciously delivered his entire lecture just for this engaged listener.

Demonstrating a continuing commitment to inclusivity, the ACA hosted a session on the #IAmRemarkable initiative, co-chaired by ACA members Sandra Gabelli and Callie Saeher, empowering participants to celebrate their achievements and counter societal norms that often discourage self-promotion, particularly among underrepresented groups. The session fostered an environment of encouragement and confidence.

The ACA recognized outstanding contributions this year by awarding over fifteen poster prizes, including the IUCr Pauling Poster Prize to Madeline M. Glennon, a graduate student from the University of Notre Dame, for her poster titled 'Structural Elucidation of an RNA Triple Helix in Complex with a Small Molecule.' Additionally, three major awards were celebrated: the Margaret C. Etter Early Career Award to Benjamin Frandsen of Brigham Young University, the M.J. Buerger Award to Thomas Albrecht-Schönzart from the Colorado School of Mines, and the Bertram Eugene Warren Diffraction Physics Award to John Greeden of McMaster University.

From left to right: Attendees enjoying the banquet, a snapshot from the poster session, and the ACA Meeting Committee addressing guests at the banquet.

For a comprehensive look at the ACA2024 program, please visit the ACA website's "Past Meetings" page. Recorded sessions will soon be available on the ACA History Portal for further insights. The ACA extends heartfelt gratitude to the 2024 Meeting Committee, poster session co-chairs, session chairs, workshop organizers, speakers, and exhibitors for making this meeting possible. And to every attendee, thank you for being part of this extraordinary global scientific community.

From left to right: From left to right: A spontaneous talk, new badges, and the 2024 SIG chairs kicking off preparations for

the 2025 program.

Mark your calendars for our 75th Anniversary Meeting, happening July 18-23, 2025, at the Westin Chicago Lombard! In honor of this diamond anniversary, we'll reflect on past meeting highlights, celebrate the field's growth, and recognize the remarkable contributions of our community. More details coming soon!

SCANZ Crystal 35 Meeting Report – Going West!

Christopher Sumby, The University of Adelaide

Crystal35, the 35th Biennial Conference of the Society of Crystallographers in Australia and New Zealand (SCANZ), was held from the 27 - 29th October 2024 in Fremantle, Western Australia. The Crystal meetings tend to be held in the state where the SCANZ president resides, and this was no different, bringing us back to Western Australia for the second time in seven years for a meeting organised by Prof. Charlie Bond and a team of local and interstate crystallographers and structural biologists. Crystal35 was held in Fremantle (Walyalup, the local Nyoongar peoples' name for the area), a seaside suburb of Perth. While close to Perth and Perth airport, Fremantle is a charming destination full of narrow streets lined with heritage buildings, close to historical and functioning dock areas, with great access to well-known local breweries and cafes.

Once again, the meeting was an excellent size for networking and scientific discussions, attended by 128 attendees, and was a fantastic opportunity to catch up with much of the Australian and some of the New Zealand crystallographic community. Despite being a significant distance, the meeting was attended by a small contingent of New Zealand crystallographers, as well as international speakers from Japan, Singapore and South Africa. The organising committee of Charlie Bond, University of Western Australia (UWA), Chair, Mihwa Lee, University of Melbourne, Stephen Moggach, UWA, Joel Haywood, Curtin University, Rhys Grinter, Monash University, Stephanie Boer, ANSTO, Gemma Turner, UWA, Luke Smithers, UWA, and Crystal Cooper, UWA developed a vibrant and diverse program with 21 invited speakers and a series of concurrent sessions with speakers selected from abstracts.

Highlights of the program included the 1987 Fund Lecture by Prof. So Iwata (Kyoto University), the awarding of the 2023 and 2024 Sandy Mathieson Medals to Prof. Neeraj Sharma (UNSW) and Prof. Jack Clegg (University of Queensland), respectively, and the 2024 Lawrence Bragg Medal to Prof. Jenny Martin (University of Queensland and Griffith University). Prof. Iwata gave an excellent talk on time-resolved (4D) structure analysis of membrane proteins and its application to drug discovery. This included a discussion of the structures of membrane proteins, mainly GPCRs and transporters, and investigation of the complex structures of the receptor sites, which can be used for drug discovery.

Left to right: Prof. Charlie Bond, SCANZ President, presenting the Bragg Medal to Emeritus Prof. Jenny Martin, the 2024 Sandy Mathieson Medal to Prof. Jack Clegg, and the 2024 Sandy Mathieson Medal to Prof. Neeraj Sharma. Photos by Chris Sumby.

Prof. Sharma was the 2023 recipient of the Sandy Mathieson Medal, awarded for distinguished contributions to science involving X-ray, neutron, or electron diffraction and/or imaging by a researcher within 15 years of the award of their PhD (link). Prof. Sharma investigates the structure and function of batteries using synchrotron and neutron diffraction techniques, and gave us a talk spanning from fundamental battery science through to analysis and testing of commercial batteries, including batteries that had been subjected to a proximal explosion. Prof. Clegg presented his team's recent work on flexible or bendy crystals, which helps rewrite some

of the conventional wisdom of crystalline materials as being brittle and inflexible. Prof. Clegg showed the scope of potentially flexible materials, including the use of advanced single-crystal synchrotron measurements to understand the mechanism of bending and the location of the stored forces in these crystals.

The final named lecture, given on the final day of the meeting, was the Bragg Medal award for distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging by Prof. Martin. Prof. Martin gave an engaging presentation starting from William Henry and William Lawrence Bragg and spanning her time in crystallography, including the early use of scientific computing, cakes inspired by crystallography and structural biology, and her contributions to gender equity and diversity in SCANZ and the IUCr.

A diverse group of keynote lecturers provided excellent coverage of all aspects of crystal growth and structure determination, including talks titled “CryoEM structures of the multimeric secreted NS1, a major factor for dengue hemorrhagic fever” (Prof. Shee-mei Lok, Duke-NUS Medical School, Singapore), “Predicting crystal growth and morphology from accuracy to speed” (Prof. Julian Gale, Curtin University), “Crystal engineering with multicomponent crystals” (Prof. Delia Haynes, Stellenbosch University, South Africa), and “TRAPped in an elevator: amino-sugar uptake and utilisation by bacteria” (Prof. Renwick Dobson, University of Canterbury, New Zealand).

Two excellent poster sessions were held, one at lunch on Sunday and the second in the evening on Monday, with 42 posters displayed over the course of the three days. Lots of discussion took place as presenters vied for five poster prizes, which were awarded at the close of the conference. Other highlights included the Rising Stars session, a lunchtime session hosted by beamline scientists from the Australian Synchrotron on the new beamlines (MX3, ADS and BioSAXS) coming online as the BRIGHT program reaches completion. The Rising Stars of the conference were Dr Charles Bayly-Jones (Monash University), Dr Isabelle Jones (Curtin University and UWA), Dr Katherine Davies (The Walter and Eliza Hall Institute of Medical Research and Melbourne University), Dr Hunter Windsor (UNSW) and Dr Rebecca Frkic (Australian National University).

The Rising Star session presenters bookended by the session chairs Dr Joel Haywood and Dr Josie Auckett (left), and the poster prize recipients with Dr Crystal Cooper and Prof. Charlie Bond (right). Photos by Chris Sumby.

Crystal35 also provided an opportunity for a SCANZ business meeting. The focus of the meeting was changes to the SCANZ constitution to complete some steps to modernise it and to provide greater structure, certainty around the council terms, the timing between Crystal meetings, and the addition of a new standing committee for outreach. The leadership of SCANZ now passes to the new president, Prof. Chris Sumby (the author of this article) from the University of Adelaide, with the new vice-president being Prof. Emily Parker (Professor of Chemical Biology at Victoria University of Wellington and Science Advisor to the MBIE, Ministry of Business, Innovation and Employment in NZ) and a committee comprising Prof. Charlie Bond (past president), Assoc. Prof. David Turner (secretary), Prof. Jack Clegg (treasurer), Dr Michelle Miller (newsletter editor), and committee members Dr Lauren Macreadie, Dr James Hester, and Prof. Stephanie Gras. Further representation also comes via the National Committee for Crystallography (NCCr) representatives in Australia and New Zealand. At present, this includes Prof. Kurt Krause from Otago University the NZ NCCr representative with the Australian role vacant.

Crystal35 was bookended by two excellent social events, with an informal mixer at the Ball & Chain, a restaurant and bar attached to the conference venue, on Saturday night and a conference social at the Gage Roads Brewing Company on the Tuesday night. Many participants also took the opportunity to visit Rottnest Island, a 25-minute ferry ride from Fremantle, to see quokkas, a small wallaby-like marsupial, and to experience the stunning scenery of this protected nature reserve.

Clockwise from top left: Little Creatures brewery in Fremantle (photo: Chris Sumby), the pre-conference mixer at the Ball & Chain (photo: Charlie Bond), the conference venue (the Esplanade Hotel) (photo: Chris Sumby) and the conference social at Gage Road Brewing Company (photo: Charlie Bond).

Results of the 7th CSP Blind Test Published - Overcoming Pharmaceutical and Other Materials Issues Before They Exist

Author not stated in source

Two scientific papers have been published detailing the findings from the 7th Crystal Structure Prediction (CSP) Blind Test. To coincide with these publications, the Cambridge Crystallographic Data Centre (CCDC) has released a CSP Blind Test database containing 171,679 entries from 207 different landscapes.

CSP predicts the most likely crystal structures to form from a given molecule, based on its 2D chemical structure. Most methods use informatics and computational science techniques. Predicting more stable structures leads to many benefits including improved manufacturing processes, patent protection and breaking, and the potential discovery of new, improved materials. Read more.

BioChemGraph - CSD Data Linked to PDBe, ChEMBL, and Other Sources via UniChem

In the era of data-driven biology, integrating information from different resources is essential yet often challenging. The BioChemGraph project addresses this challenge by creating infrastructure that consolidates structural, functional, and biochemical annotations for small molecules and their targets from key resources: the Protein Data Bank (PDB), the ChEMBL database, and the Cambridge Structural Database (CSD). Read more.

How to Compare the Packing of Your Polymorphs

Polymorphism is the ability of a compound to crystallize into multiple forms, which is important for pharmaceuticals since different polymorphs can affect a drug's bioavailability and efficacy. Comparing polymorphic structures can be complex, but tools like Crystal Packing Similarity and Structure Overlay in Mercury can help identify differences and similarities by examining packing environments and conformations. Read more

Check out all our blogs here.

New video: Unlock crystal structure secrets with Mercury

This 5-minute video demonstrates how to use the Powder Pattern Simulator in Mercury. The Simulator is compatible with both CSD entries and structures in CIF format. Users with a CSD-Core license or higher (such as CSD-Materials, CSD-Discovery, or CSD-Enterprise) have access to the option of adding a second wavelength in the simulation. Watch now.

Events

In 2024, we hosted six free virtual workshops, attracting over 650 attendees from 61 different countries. Over 200 attendees achieved a perfect score of 100% on the post-workshop test. Thank you to everyone who joined us! We are preparing more virtual workshops for next year, with confirmed dates on the 11th and 25th of March and the 8th of April 2025.

The topics for these workshops will be announced soon, so please keep an eye on the events page of our website for updates or sign up for the CCDC newsletter to be the first to receive event announcements.

If you would like to suggest topics for our workshops, webinars, and CSDU online training modules in 2025, please email us at hello@ccdc.cam.ac.uk.

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Setting the Pace in Non-Ambient XRD: A New Benchmark for Environmental Heating

Author not stated in source

Pioneers in non-ambient X-ray diffraction

While most X-ray diffraction measurements are performed under ambient conditions (i.e. room temperature, ambient pressure), many processes, e.g. geological, catalytical or industrial ones, occur under non-ambient conditions. Non-ambient parameters, such as temperature, pressure, humidity or different gas atmospheres, can significantly alter a material's structure, property or reactivity. Since many of these changes are reversible, or occur stepwise with multiple intermediates, in-situ investigation of materials under non-ambient conditions is an essential tool in establishing a detailed understanding of a material's properties.

When we introduced the HTK 10 High-Temperature Chamber at Anton Paar back in 1964, we made our mark in the history of non-ambient X-ray diffraction. The HTK 10 High-Temperature Chamber was capable of heating samples up to 1,600 °C in order to study their structural changes by X-ray diffraction during heating.

Prior to this, non-ambient X-ray diffraction of various materials was mainly done with homemade equipment, and there was no real commercial heating chamber available on the market. This changed when we entered the market 60 years ago. Since then, our knowledge and experience in X-ray diffraction - especially under non-ambient conditions - has steadily grown. This has led to our current broad portfolio of non-ambient X-ray diffraction attachments for studies between -190 °C and +2,300 °C under different atmospheres (dry and humid) and pressures, as well as mechanical or electrical loads. Along with this complete portfolio, we also create customized solutions for our customers - something that has made Anton Paar the market leader in non-ambient XRD.

This year, we're proud to announce the launch of the HTK 1500 High-Temperature Chamber, the new benchmark of environmental heaters for high-temperature X-ray diffraction. The HTK 1500 allows for homogeneous heating of all types of sample materials, including crystalline powders and bulk samples, up to 1,500 °C. This makes it the only true environmental heater available on the market that reaches such high temperatures without any compromises in precision. The temperature sensor is located directly beneath the sample in a protective ceramic holder, guaranteeing highly repeatable and reliable temperature measurements. A fast and easy switch between reflection and transmission modes, by the use of a capillary extension, makes the HTK 1500 suitable for air-sensitive and organic powders and liquids. Sample spinning is also provided, which is crucial for improving data quality by overcoming preferred orientation. The sample carriers are made of chemically inert alumina, minimizing the risk of reactions with samples, even at high temperatures. A user-friendly slider for the sample holder allows for quick and reproducible sample exchange.

The HTK 1500 is completely compatible with Anton Paar's XRDynamic 500 X-ray diffractometer. This combination offers high automation, including stage recognition, stage and sample alignment and realignment during heating, and easy connection of cooling water, vacuum, and gas lines. The seamless integration into the XRDynamic 500 control software ensures a user-friendly experience for high-temperature XRD analysis.

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TRIBUTE TO THE SUPPORT GROUPS IN THE QUASICRYSTAL DISCOVERY – A 40-YEAR ANNIVERSARY

Istvan Hargittai

Forty years ago, in 1984, a brief communication in Physical Review Letters announced the discovery of quasicrystals (not yet using this term). Three scientists joined Dan Shechtman as co-authors. Previously, associates of the then National Bureau of Standards assisted Shechtman in his experiments. In 2011, Dan Shechtman received the Nobel Prize in Chemistry for the discovery of quasicrystals. There was no doubt that he deserved it and that he deserved the prize unshared. This personal review is dedicated to his "support cast," the members of two groups that assisted his discovery and the publication reporting it.

Dan Shechtman, 1995, in the author's home in Budapest. Photograph by Istvan Hargittai

Dan Shechtman's unshared Nobel Prize in 2011 was unequivocally appreciated by those familiar with his milestone discovery and his perseverance during the preceding years. Great scientific authorities had questioned the validity of the interpretation of his observation. The award signaled the official seal of approval of the existence of quasicrystals, which he announced in 1984 [1] but had observed in 1982 (see, eg, [2−7]).

In 1981, Dan Shechtman of the Technion—The Israel Institute of Technology—went for his first sabbatical at the National Bureau of Standards (NBS; today, the National Institute of Standards and Technology, NIST, in Gaithersburg, Maryland). John W. Cahn (1928−2016), a senior scientist at NBS initiated his appointment. The two first met in the late 1960s when Cahn visited the Technion, where Shechtman was an engineering student in the Department of Metallurgy. At the time, Cahn was already well known for his thermodynamics of materials [8]. Their next meeting was in 1972 when Shechtman was a postdoctoral fellow at the Aerospace Research Laboratories, Wright-Patterson Air Force Base, near Dayton, Ohio.

John W. Cahn, 1995, in Gaithersburg, Maryland, photograph by Istvan Hargittai

Their "life-changing" meeting [8] happened in 1979 when Cahn and his wife stayed at the Technion for a longer period. By then, Shechtman had become an expert in electron microscopy and developed a method for studying metallic powders by transmission electron microscopy. His research focused on rapidly solidified metallic alloys, something a group at NBS had also been working on but not very successfully. Cahn thought that Shechtman would be a good addition to the group and invited him for a talk and then for a stay at NBS. Shechtman at NBS was supported by a joint program of the Defense Advanced Research Project Agency (DARPA) and the National Science Foundation (NSF). He had freedom in choosing and executing his research projects.

Shechtman first visited NBS in the summer of 1980 and gave a talk. Then, he returned with his family in August 1981 for "two magnificent years" [8]. 1995 he remembered: ''I started by studying rapidly solidified aluminum-iron alloys. I analyzed the phases present and the solidification patterns. I collaborated mainly with members of the metallurgy group, Bill Boettinger, Bob Schaefer, and Frank Biancaniello. We wrote a series of papers together and understood rapid solidification better. It was in April 1982, half a year after I had arrived, that I discovered the icosahedral phase'' ([2], p. 84]).

In 1984 at NBS, from left to right: Frank Biancaniello, John W. Cahn Denis Gratias, Leonid Bendersky, Dan Shechtman, and Robert Schaefer. Photograph by H. Mark Helfer/NIST; courtesy of NIST (colorized by the Editor).

Frank Biancaniello's role was especially important in Shechtman's studies. He was a technician, not yet a full-fledged researcher at the time (as he became soon afterward); his tasks included the preparation of the alloy samples of various compositions for the electron microscope–electron diffraction experiments. According to the other members of the group, Biancaniello was most enthusiastic about this project. He was happy to work many extra hours, including nights and weekends, and he was as skilled as he was devoted to this work. At Shechtman's initiative, the tests extended even outside the range of reasonable compositions—reasonable, that is, for expected practical applications. Biancaniello remembered [9]:

‘‘Obviously, the quasicrystal discovery was the most important one culminating in Danny’s Nobel. But many other exciting projects we worked on came to fruition over the years. I’m sure you have heard of some of the bulk metallic glass research being carried out over the years, with yield strengths on the order of 1 to 2 gigapascals with no ductility. Steve Ridder and I developed a High Nitrogen Stainless Steel with a yield strength of 1.1 gigapascals with an elongation of 60%, using so-called rapid solidification technology. I only mention this in an attempt to demonstrate how intellectually stimulating these thirty years were starting with working with Danny Shechtman and continuing on to recent times. As Bill Boettinger mentioned, we worked on many projects with Danny. Steve Ridder and I did more recent research with Danny using a quasicrystal for a wear-resistant coating while doing thermal spray studies.’’

Shechtman narrated in our 1995 conversation about some of the details of the seminal experiment ([2], p. 84):

“At first, I was studying rapidly solidified aluminum-iron alloy, which we thought had some commercial future. Eventually, it turned out that although rapid solidification research resulted in several useful products, it did not develop into a widespread technology. This, however, is not important for our story. In the aluminum-iron binary system, there was one metastable phase, Al6Fe, which I studied. The equivalent Al6Mn in the aluminum-manganese system is a stable phase, and I wanted to compare some crystallographic features of the two. We started, therefore, to produce a series of aluminum-manganese alloys with increasing amounts of Mn in them. Eventually, I ran wild, from a practical point of view, since beyond several percent of manganese the rapidly solidified alloy becomes brittle and therefore useless. Among the alloy ribbons that I have prepared with Frank Biancaniello by melt spinning, there were alloys which contained over 25 weight percent manganese. On April 8, 1982, as I was studying by electron microscopy rapidly solidified aluminum alloy which contained 25% manganese, something very strange and unexpected happened. It is worthwhile to look at my TEM [transmission electron microscope] logbook records of that day. For plate number 1725 (Al-25% Mn) I wrote: ‘‘10 Fold ???’’ There were ten bright spots in the selected area diffraction pattern, equally spaced from the center and from one another. I counted them and repeated the count in the other direction and said to myself: ‘There is no such animal’. In Hebrew: ‘Ein Chaya Kazo’. I then walked out to the corridor to share it with somebody, but there was nobody there, so I returned to the microscope and, in the next couple of hours, performed a series of experiments. Most of the needed experiments were performed at that time. A few days later, all my work was complete, and everything was ready for the announcement. Then it took two years to publish it.”

This comment that “it took two years to publish it” signified a hard time for Shechtman. The delay was not only due to the disbelief of the scientific community that the dogma about the impossibility of fivefold symmetry (and other ‘‘forbidden’’ symmetries) in the world of crystals should fall. It was also that no convincing model could be constructed for interpreting the unexpected observation. At the same time, sitting on a seminal observation, he felt the necessity of communicating it to the broader community of researchers. He produced a manuscript in co-authorship with Ilan Blech (b. 1936), one of his former professors at the Technion, who devised a model to interpret Shechtman’s observation. This also meant that in Ilan Blech Shechtman found someone who shared his conviction that it indeed was an observation of a heretofore unknown structure.

They submitted their manuscript to the Journal of Applied Physics (JAP) in the summer of 1984. The disappointing editorial decision came back with a review. The Editor of JAP, Lester Guttman, wrote [10]: ‘‘Our reviewer and we both believe that your paper will not reach the most appropriate audience through this journal, and we are therefore returning your manuscript. We wish to make it clear that this is not a comment on the technical quality of your work; rather, it is an attempt on our part to try to place papers where they will be of the greatest use to the greatest number of people.’’ As the manuscript was more of the nature of a report in metallurgy than in physics, eventually, it was published in a metallurgy journal, Metallurgical Transactions [11]. The name of the journal was later changed to Metallurgical and Materials Transactions. In the wake of Shechtman’s Nobel Prize, the editor of this journal invited Shechtman’s three co-authors of the Physical Review Letters paper to recount their experience in that co-authorship [12]. This account was followed by a reproduction of the 1985 Shechtman-Blech paper [11].

Even before Shechtman received the letter of rejection from JAP, he showed the manuscript to John W. Cahn. Shechtman did not do this too eagerly, as Cahn’s initial reaction when he showed him the April 8 observation

was rather negative. In Cahn's words [13]: "One day he came into my office, and said, 'John, what do you think of a 10-fold axis?' I said, 'Don't bother me, Danny, this is clearly twinning,' and he said, 'I don't think so.' Then we discussed a number of experiments to decide this question. I didn't know much about twinning, but I did know that through twinning you could get unexpected symmetries."

They did not talk again about Shechtman's observation until mid-1984. In the meantime, Shechtman was back in Israel, and when he returned, he wanted to inform Cahn about the difficulties of publishing his April 8 observations. At the time, Cahn was attending a Gordon Conference in Aspen, Colorado, but when Shechtman's word reached him, he flew back one day early from the conference. Shechtman showed him the manuscript that had been submitted to JAP but had not been rejected yet. We continue with Cahn's own words [13]:

"I read this paper immediately and got very excited because I saw the data for the first time. I wasn't convinced by the Blech model, but I was very much convinced by the experiments. It was obvious that it was not twinning, that it was something outside of what was known. I'm sure that had I seen the data in '82, the same day when they were taken, we wouldn't have wasted two years. On Friday, I met with Danny and said, this is a poorly written paper; you're hiding this new phase. The entire paper was about experiments on aluminum–manganese. It started out by saying that we did this, we found this, and gave a list of the known periodic phases for each composition range, and buried, in half a paragraph, was a new phase, in the middle of an otherwise very conventional paper. My impression was that it was written that way to sneak it past the referee because everybody, except Blech, had told him that he had nothing. I remember that Friday going to the bosses [at NBS] and telling them that this is really something and it's going to be big. I more or less said that we should mount a major effort; lots of people should shift because this has got to be investigated. At this stage I was not a co-author, and I did not expect to be a co-author. I told Danny that this is the wrong paper, but Danny told me that the paper had been submitted."

Denis Gratias and Dan Shechtman in Shechtman's office at the Technion, in January 2011, nine months before the announcement of Shechtman's Nobel Prize. Shechtman is wearing his "quasicrystal tie." Photograph by Istvan Hargittai

When the paper was rejected by JAP and published in Metallurgical Transactions, Cahn encouraged Shechtman to write "a proper paper". To this, Shechtman said to Cahn [13]: "if you feel so strongly about it, can you write this paper?" To which Cahn replied: "Danny, this is your work; you're making me an enormous gift." Shechtman did not mind, and the two and a half journal-page paper was produced, though not before Cahn had invited a young French theoretician, Denis Gratias, to join them in writing the paper. Blech did not participate in producing this manuscript, but Shechtman added his name out of loyalty. Blech soon went into industry; he now lives in California. The others continued in research. Denis Gratias is currently a research director emeritus at the CNRS, the French National Center for Scientific Research. His highest recognition was his election to corresponding member of the French Academy of Sciences in 1994.

John W. Cahn's co-authorship in the 1984 Physical Review Letters paper was an important event, but only one of several in his rich research career. He was born in Cologne, Germany, in a Jewish family. His father was a lawyer known for his anti-Nazi sympathy who narrowly escaped arrest upon the Nazi takeover in 1933. The family fled Germany and, after a few years in Holland, emigrated to the United States in 1939. They lived in New York City, and Cahn served in the U.S. Army in Japan during its occupation. Cahn received a bachelor's degree in chemistry in 1949 at the University of Michigan and a PhD in physical chemistry in 1953 at the University of California Berkeley. For the next decade, he worked in chemical metallurgy at General Electric in Schenectady and became a professor of metallurgy at the Massachusetts Institute of Technology from 1964−1978, followed by his tenure at the NBS/NIST from 1977−2007. His research results in metallurgy, non-crystalline materials, and other areas of materials science and technology were manifested in numerous publications and named effects and equations. The development of his research interests has been summarized [14]. His achievements were recognized by numerous awards and other signs of appreciation. He was elected member of the U.S. National Academy of Sciences in 1973 and the National Academy of Engineering in 1998. He received the National Medal of Science in 1998 and the Kyoto Prize in 2011.

When Cahn accepted Shechtman's assertion that his observation was a discovery of a heretofore unknown phenomenon, however great Cahn's authority was in materials science, there were more hurdles to overcome. In Cahn's words [13]:

"At NIST, we have an Editorial Review Board. Every paper from the Institute has to be reviewed internally before it can be sent out. This Review Board was afraid of another polywater. The Bureau of Standards had been burned by polywater publications. The Board wanted to be on the right side this time and had asked local crystallographers to give them lectures about fivefold symmetry, why it can't be. They were spending a great deal of time. The Board was split. My Division Chief of Metallurgy, also an old friend, said to me, 'John, you have a wonderful reputation. Why ruin it by putting your name on something like such a paper.' I said, 'please, read this paper, it is very important and very exciting, and it's not a time to be conservative.' The Board took a very long time, they had lots of meetings, sometimes they came to me for advice but I was never present at these meetings. They carried an inquiry very carefully, and eventually they approved the paper. Finally, in mid-October, we could send off the manuscript. It came out three weeks after it was submitted."

After the paper was published, it generated enormous interest and an avalanche of publications. The foremost among them was the brief communication by Paul Steinhardt and Dov Levine of the University of Pennsylvania. They offered a plausible model and coined the name quasicrystal [15].

As we have seen Shechtman had two supporting teams, one each for his seminal experiment and for its publication, with John W. Cahn bridging the two. The following years, however, Shechtman spent essentially as a lone hero of perseverance. There was a growing number of his supporters, but the dissenters could refer to the devastating opinion of Linus Pauling (1901−1994), arguably the most revered chemist of the time. In the fall of 1993, not long before his passing, I asked Pauling about quasicrystals. He dismissed it; not the experiment, not even the name, but the interpretation, and he did this in an uncompromising manner [16], "As to the quasicrystals, you know that I contend that icosahedral quasicrystals are icosahedral twins of cubic crystals containing very large icosahedral complexes of atoms. It is not surprising that these crystals exist. The first one to be discovered was the MgZnAl compound reported by my associates and me in 1952. We did not observe quasicrystals of this compound, but they have been observed since then." Even after Pauling's death, many of his followers were reluctant to disrespect the memory of their Master by accepting Shechtman's discovery for what it was. The Nobel Prize in 2011 ended any such hesitation.

On November 3, 2011, at NIST, from left to right Istvan Hargittai, William Boettinger, Frank Gayle, Francis Biancaniello, Stephen Ridder, Leonid Bendersky, Robert Schaefer, and Balazs Hargittai. Photograph by Istvan Hargittai.

Although solid state structures have not been in my research interest except for comparison with gaseous structures, quasicrystals have fascinated me ever since I heard about them. Curiously, I had learned about the possibility of their existence as early as 1982. I organized a lecture series for Alan L. Mackay of Birkbeck College at Eötvös University in Budapest and two of his presentations were about fivefold symmetry. Mackay warned us that if we believed the impossibility of fivefold symmetry in solid-state structures, as classical crystallography had taught us, we might let it pass us unrecognized even if we observed it (see, eg, [17, 18]).

In 1987, I attended a crystallography meeting in Moscow in honor of Alexei Shubnikov's centennial [19]. There, Shechtman's discovery dominated the discussions in the coffee breaks. We met first in person in the early 1990s when I spent a month in Israel as a visiting professor at Ben-Gurion-University in Beer Sheva. This stay allowed me to give invited lectures at all major universities in Israel. During one of these presentations as I was talking at length about the significance of Shechtman's quasicrystals, suddenly someone in the audience stood up and said: "I am Danny Shechtman." Thus, our friendship began. In 1995, I was responsible for the scientific program of a crystallography meeting/school in Balatonfüred, Hungary, and quasicrystals received plenty of exposure with Shechtman as a star lecturer. There were other encounters but fast forward to January 2011 when at my initiative and, perhaps, at others' as well, there was a meeting at the Technion celebrating Shechtman and his discovery. This meeting happened nine months before the announcement of his Nobel Prize.

My son, Balazs, and I visited NIST on November 3 and 4, 2011, responding to an invitation for a presentation about Edward Teller and the other Hungarian “Martians” of science. As our visit happened a few weeks after the announcement of Shechtman’s Nobel Prize, I gave an impromptu talk about the quasicrystal discovery as well. We spent several hours with Shechtman’s former colleagues, and we learned about their warm feelings they had toward Shechtman and their pride for having contributed to the discovery [5].

His former NIST colleagues have rarely figured in Shechtman’s statements. In his two-minute speech at the festive Nobel banquet on December 10, 2011, of his two support groups, he mentioned only the names of his co-authors of the seminal paper [20]. There was no acknowledgments section in his Nobel lecture [21], which my wife and I attended in December 2011 in Stockholm. Neither was there one in his Gregory Aminoff lecture in 2000 in Stockholm, which we also attended. The latter was linked to the “Symmetry 2000” conference. Alas, Shechtman did not produce his presentation for the volumes of the proceedings of that meeting [22], just as he never wrote up his Nobel lecture for publication either (it can be watched as a video [21]) . One can only speculate that he may have had some frustrating experience at NBS that he did not wish elaborating. He had acknowledged though his joint work with NBS associates in our 1995 conversation when he told me: “I collaborated mainly with members of the metallurgy group, Bill Boettinger, Bob Schaefer, and Frank Biancaniello” ([2], p. 84].

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