

# IUCr

## Newsletter Archive



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## President's Letter

*Santiago García-Granda*

The 75th anniversary of the IUCr marks a turning point in our organization, when we still have a close memory of our origins and the people who have built the International Union of Crystallography, both from our personal experience and the references of many colleagues. This August, we had our 26th assembly and the annual conference of our Union, where we enjoyed our history told by some of its protagonists. Many of our referents are no longer with us; very recently two of our former presidents passed away, we lost Professor André Authier earlier this year, and even closer is the death of Professor Henk Schenk. Many other crystallographers of our community left us in these 75 years of history, and all of them deserve our recognition and our loving memory.

Although we stand on the shoulders of giants, we are facing a very different world from that of our first General Assembly in 1948. That is why it is so important that we invigorate and adapt our organization to face the future with confidence and renewed enthusiasm. The process that begins in Melbourne is essential to define our Mission, Vision, and Values in an open and participatory way; we must find the keys that will allow us to face, with the new generations, women and men, the new challenges to continue developing and leading structural science in a very different world. The results of the consultation and discussion will help the new Executive Committee make the right decisions to ensure the scientific and social leadership of Crystallography and Structural Science for the remainder of the 21st century.

The IUCr must keep going on and reinforce the initiatives started almost 10 years ago, on the occasion of IYCr2014, focusing on: (i) Education, to provide new generations of crystallographers and structural scientists; (ii) Research, by fostering scientific collaboration and leadership in Structural Science through the commissions and our journals and books; (iii) New generations, creating a young division to attract the early-career scientist to have a strong voice in and from the IUCr; (iv) Society, by reinforcing the impact of Crystallography on society so as to obtain the support of stakeholders and put Crystallography and Structural Science on the agenda of the decision makers; (v) Organization, favoring the links between the regional associations, boosting their influence within the IUCr, and reinforcing our team in the Chester Office; (vi) Promotion, keeping the momentum and favor gender equality at all levels and activities; (vii) Attraction, extending the family with child-friendly Crystallographic conferences.

After the 2014 IYCr, the IUCr has been more active in demonstrating, fostering, and coordinating the impact of Crystallography and Structural Science on humanity, thus providing networking between scientists worldwide and having an active role in the ISC. The experience with the successful hybrid IUCr25 in Prague, offers new opportunities to adapt the IUCr to the new environments.

Our organization has grown in its geographical presence with the latest addition of AfCA, the African Crystallographic Association in the Melbourne General Assembly, completing the five regional Associations that make up the IUCr. These regional branches of the Union will contribute to bringing science to new emerging countries where Structural Science is less developed and will allow for a more diverse voice to be heard from crystallographers all over the world, without exception. The collaborative projects being developed with governments, companies and non-governmental organizations will give an extraordinary boost to the development of science in all regions of the world. The Light Sources for Africa, the Americas, Asia and the Middle East Project (LAAAMP) is one of them.

This Newsletter is a great tool to bring our community together, being a meeting point for philosophical discussions, not only on scientific issues, but also on issues that affect our societies and the planet, contributing effectively to the discovery of our disciplines by the global society and giving us the possibility to disseminate our activities worldwide. Many thanks to Mike Glazer and Andrea Sharpe and all contributors.

We must be able to maintain the bonds of scientific collaboration above conflicts and align ourselves with the progress of global society in terms of peace, justice and equity, diversity, and sustainability. We have to ensure that future generations have the resources and conditions to sustain life on the planet, and this is not only for the human species but also to maintain the planet's biodiversity and the wildlife.

It was very good to be back in Australia 36 years after the well-remembered 14th IUCr 1987 Perth congress. The scientific programme was excellent; the setting, the facilities, the organisation, and the human atmosphere was perfect, managing to regain a sense of normality after our extraordinary experience in Prague. The participation of young scientists with excellent lectures put us in the best possible scenario for the future. The lecture of our Ewald laureate, Prof. Wayne Hendrickson, led us through many years of the development of anomalous dispersion and its extraordinary influence on the development of Macromolecular Crystallography. The consolidation of new methodologies such as 'Alpha Fold' has revolutionised our methodologies and the emerging development of Artificial Intelligence opens new and unimaginable future challenges for Structural Science. All of this was complemented by an ambitious programme for the social integration of our discoveries and the attraction of scientific vocations from the earliest ages, which will help ease the imbalances in science and technology. Many thanks to SCANZ (Society of Crystallographers of Australia and New Zealand) and to its President, Prof. Charlie Bond, for inviting us to Melbourne. Thank you very much indeed to the organisers of the 26th Congress and General Assembly, to Professors Michael Parker, Brendan Kennedy, and Megan Maher, and also many thanks to all the Melbourne team. You made us feel at home. Thanks to the sponsors and to the participants, and thanks to all of you who made this Congress and the IUCr possible.

I am very happy that my election as the 27th president of the IUCr was in Melbourne, in Australia, and at the heart of this magnificent conference and superb scientific framework, especially because of the contributions of young crystallographers. After this conference, we will start a new term after celebrating our first 75 years of history together. Some of the colleagues I met in 2014 in Montreal when I joined the EC, and later, are leaving the EC after Melbourne or did before; many thanks to all of them. In particular, to the members who did so immediately after the last GA: Sven Lidin, Jennifer Martin, Masaki Takata, and Bo Iversen. Many thanks to past presidents, Marvin Hackert and to Hanna Dabkowska, who will continue as outgoing president of the new executive committee, as well as to Graciela Diaz de Delgado, our new vice-president, and I welcome the four new committee members: Trevor Forsyth, Atsushi Nakagawa, Susan Bourne, and Maria Cristina Nonato. I would like to finally mention our wise convener, Prof. Malcolm Cooper, and the members of the Finance Committee.

Last but not least, thanks must go to our IUCr team in Chester, who always work hard, especially in the conference year, and to all our sponsors, who give the necessary support to make our meetings and many of our projects feasible.

We have initiated a process to redefine our Purpose, Vision and Values. Let's do it in the next triennium. The new Executive Committee is ready to face the challenges of the Union until our meeting in Calgary in 2026.

We all must support our team in Chester; we must be aware of their needs and ensure a suitable working environment and exciting projects that will enable their professional development and make them attractive to new recruits, thus allowing for an orderly generational handover. The change of address to the UK, which is currently under study, would, if possible, improve the efficiency of our administrative processes considerably, with the consequent improvement of our activity in Chester.

One of our tasks will be to create a Young Division of Crystallographers and Structural Scientists, being the generational renovation of great importance for the Union. The input of the new generations of crystallographers and structural scientists worldwide is vital for our Union.

A critical aim will be to improve our finances and revitalise our journals; this is one of our major issues. Everybody, the Chester production and marketing team, together with the journal Editor-in-Chief and his team, should work towards making our journals more competitive. But not only them: our Scientific Commissions must play a key role in the development of our editorial work and so must our regional and national committees and each crystallographer by publishing his/her results in an IUCr journal.

The IUCr is in continuous evolution, and in this triennium, with the help of the new EC, the Chester Office, and with your support, our task is to maintain, revitalise, and renew our activities, redefining our Mission, Vision, and Values, as well as to maintain the highest scientific and social impact with IUCr Meetings in Calgary 2026 and Berlin 2029, as was the last one in Melbourne.

We will work to maintain our excellent partnership with our Associated Companies in order to achieve the best possible integration of projects of mutual interests, generating constant interactions to establish a fluid relationship of trust necessary to tackle new initiatives.

We stand at the service of all IUCr members and humbly ask for your full commitment with your Union.

All of us are necessary to maintain the IUCr strong, particularly the Regional Associations, the IUCr Commissions and Committees, Editors, Co-editors, Referees and Authors of our journals, and all individual crystallographers, women, and men, collaborating in the best scientific and human environment. It's important for us that you feel comfortable in our Union and be proud to belong to the IUCr.

Many thanks to all for keeping the IUCr at the front of Structural Science.

## Editorial

*Mike Glazer*

Many of us have now returned to our home countries after attending the IUCr Congress in Melbourne. I hope that everyone found it both enjoyable and, even more importantly, scientifically fruitful. Having attended every IUCr Congress since 1966 (apart from the Prague meeting, which I watched remotely), I can look back and think about the value of these big international meetings that we hold every three years. Obviously, they provide an opportunity to learn about new science by listening to the talks and looking at the posters. But it also enables us to meet with each other, sometimes seeing old friends but also making new acquaintances. And often, this leads to new scientific collaborations. This is why the Congresses matter. In the Melbourne conference, in particular, a considerable effort was made to advertise our subject to the general public through a superb talk by Jenny Martin: "How I fell in love with Crystallography and why you should too!" (this can be viewed at .....). In addition, school children were invited to learn about crystallography through talks specifically aimed at them with the chance to see and play with several crystal models. Part of this involved everyone helping to construct the largest crystal model ever made. You can read some more about the Congress in an article by Chris Sumby (ref). I hope to have further details in the next issue of the Newsletter.

In the last issue, I mentioned the then-upcoming Oxford Hatfest. I am pleased that Marjorie Senechal has written us a report of that meeting (ref) where you can see just how much excitement was generated by the discovery of a single shape that could be stacked together, leaving no gaps but also not having periodic symmetry (at least in our 3-dimensional world!). While obviously a rather exotic bit of the mathematics of symmetry, one question I would raise is this: are there any actual crystals out there that have this kind of aperiodic structure? Start searching: a possible Nobel Prize may await you!

For crystallographers, it is essential that they learn about the concept of symmetry and how it applies to crystals. The MathCryst Commission of the IUCr performs a valuable service in this regard through holding regular schools in different parts of the world. These are led mainly by Mois Aroyo and Massimo Nespolo together with other instructors. The latest school was held in Nancy and is described here (ref).

Now, while it is the case that the concept of symmetry lies at the heart of our understanding of crystals and their structures, it should be emphasised that this is a concept that only really applies to a so-called infinite ideal crystal. Such a crystal does not exist, as in reality there are all sorts of defects and disorder always present, plus the crystal surfaces. Nonetheless, an understanding of symmetry is an essential starting point for describing crystal structures and their physical properties. If symmetry were all there were to a crystal, then I think it is fair to say that none of us would exist. Sometimes it is said that "symmetry is death." This makes sense because true symmetry is by definition, unchanging and frozen, and therefore has nothing to say about any progress or development. It is the breaks in symmetry that are responsible for the world we live in. Every

new discovery can be thought of as symmetry breaking. But to understand the breaks, one needs first to understand symmetry itself. I often illustrate this idea by playing some awful music to my students. I start with a set of repeating notes, i.e., highly symmetric and periodic, showing that such “music” soon becomes boring (see upper line in the Figure).

However, if, along the way, we introduce two or three different notes (lower line), this immediately captures our attention. Admittedly this is still not great music but it does serve to illustrate the effect of symmetry breaking. So, symmetry on its own is boring! I often upset the “crystal healing community” who sometimes contact me by pointing out that crystals are the “deadest” things in the universe! Now, having said that, symmetry does mean that crystals are very pretty and in this vein Istvan and Magdolna Hargittai have written an entertaining article entitled “Crystals Humanized” (ref).

Another way by which the beauty of Crystallography is brought into the public square is through the holding of crystal growing competitions. Here, school children are given the necessary chemical agents and learn how to grow crystals from solution. The best crystals are then judged for quality and size. In this issue, we have reports from Canada and the USA of the latest crystal growing competitions. (refs).

As ever, as Editor I have the sad task of reporting the deaths of fellow crystallographers. John White (ref) from the ANU, Canberra, was well known for his work in neutron scattering. Raimond Ravelli, was a well known structural biologist working in Grenoble, and Bruce Forsyth, a neutron scatterer. And then very recently we heard of the death of Henk Schenk, President of the IUCr from 1999 to 2002. I hope we shall have an obituary for him in the next issue of the Newsletter. I well remember his lectures on the crystallography of chocolate!

## **The Long Road to Melbourne, Australia – the 2023 IUCr Congress**

*Christopher Sumbly, The University of Adelaide*

The Melbourne skyline by night, overlooking the Yarra River, with part of the Melbourne Convention and Exhibition Centre on the bank to the right. (Photo credit Chris Sumbly).

Six years after successfully bidding for the International Union of Crystallography (IUCr) Congress, the Society of Crystallographers in Australia and New Zealand recently hosted the 26th Congress in Melbourne, Australia. The meeting was held in the Melbourne Convention and Exhibition Centre over seven and a half days between the 22nd-29th August 2023, attracting nearly 1800 participants (including 402 early career researchers) from 66 countries. The path to Melbourne was a long one in many ways, in part for the organisers who had to deal with several uncertainties during the organisation, and for many of the participants who had to make their way to Melbourne from places as far away and as diverse as Albania and Venezuela.

Australia was the host to the International Union of Crystallography (IUCr) Congress for the second time. The first instance was the 1987 IUCr Congress held in Perth in Western Australia, a meeting that left a significant legacy in Australia regarding crystallography. For the 2023 event, the organisers did a fantastic job of promoting Australia and the meeting via Twitter, the IUCr newsletter and E-Zines, promising the opportunity to experience a meeting that showcased Melbourne’s culture and Australia’s unique landscapes, and highlighted the vibrant local scientific community that has made remarkable contributions to crystallography. In addition to showcasing Australian and New Zealand science, the meeting was also to serve as a meeting point for the world’s crystallographic community, who hadn’t been able to meet in person as one since 2017 (noting the mostly virtual 25th IUCr Congress in Prague in 2021), and to allow attendees from various countries to gather to exchange knowledge, foster collaboration, and celebrate the recent breakthroughs in the field of crystallography.

The final moments before 6 years of hard work gets underway. (Photo credit 26th IUCr Congress, SDP Media)

Two days of Pre-Congress Workshops kicked off on Monday 21st August 2023, with workshops covering topics ranging from “Next-generation atomistic-level structural modelling...” to “CCP4/CCP-EM” and “Using the CSD to go from data to discoveries”. These comprehensive sessions brought together experts and newcomers alike to delve into the latest developments, technologies, and methodologies in crystallography.

The Congress officially started on Tuesday afternoon with an inspiring opening session, headlined by the award of the 13th Ewald Prize to Prof. Wayne Hendrickson who spoke on the refinement of crystal structures at ultralow resolution using approaches such as AlphaFold modelling. Delegates were welcomed to Melbourne by the Congress Chair, Prof. Michael Parker and indigenous performers from Australia and New Zealand. The opening session not only marked the commencement of the Congress but also celebrated the spirit of scientific exploration and collaboration that are hallmarks of the global crystallography community. The opening lecture was followed by the Congress Welcome Reception, which was held in the IUCr 2023 Exhibition Hall. Delegates were able to catch up with friends and colleagues, enjoy a drink, free-flowing oysters and cheese, and have the opportunity to “network” with some of Australia’s native animals.

Experiencing the fauna of Australia at the Congress Welcome Session. (Photo credit 26th IUCr Congress, SDP Media)

The Congress got under way in earnest on Wednesday with up to 12 parallel sessions available throughout the meeting. In addition to the presentations of various awards and a medal, including the Ewald, Bragg and Struchkov prizes as well as the Gjonnes Medal, there were three plenary lectures and 35 keynote lectures throughout the Congress. In addition to the award of the Ewald Prize to Prof. Hendrickson, the Bragg and Struchkov Prizes were awarded to Prof Arkadiy Simonov (development of the three-dimensional difference pair distribution function (3D- $\Delta$ PDF) approach) and Dr Robert Fayzullin (high-resolution X-ray diffraction crystal structure determination) and the Gjonnes Medal to Prof Jian-Min Zuo (contributions to the development and application of quantitative electron diffraction).

While the Congress was in-person, most of the plenary and keynote lectures were recorded and made available online, making the Congress accessible to members of the world community who could not travel to Melbourne. These included the plenary lectures, with the first two given by Prof Hideo Hosono and Dr Junko Yano on Friday and Saturday nights, respectively. Throughout the meeting, there were 120 microsymbiosia representing all the Commissions of the IUCr. This provided all participants with an abundance of talks covering a wide spectrum of topics, ranging from fundamental crystallography principles to groundbreaking discoveries.

For the first four full days of the Congress, coffee breaks and lunches were held in the large IUCr Exhibition Hall amongst exhibition booths for the 42 sponsors and exhibitors of the meeting. This ranged from Rigaku Oxford Diffraction, having a networked MicroED instrument that participants could use to collect data on a pre-loaded sample, through to the Cambridge Crystallographic Database running their CSD Leaderboard. The food was plentiful and easily accessed at the fully catered lunches, and a healthy mix of fruit was provided throughout the meeting. The large poster sessions were spread throughout the Exhibition and adjacent to the rooms used for the concurrent sessions.

In addition to the scientific program, three sessions of the General Assembly of the IUCr were held to transact the business of the IUCr as the organisation reached its 75th anniversary. Among a range of decisions made was the official recognition of the African Crystallographic Association (AfCA) as the 5th regional associate of the IUCr, the awarding of the 28th IUCr Congress to the German Crystallographic Association (Berlin, Germany, following the 27th Congress in Calgary, Canada), and the election of a new IUCr Executive Committee under the leadership of Professor Santiago García-Granda (University of Oviedo, Spain) as IUCr president.

Another highlight of the meeting was the excellent outreach opportunities associated with the Congress, including the Crystal-A-Con day on Friday 25th, and Saturday 26th of August. This event was spearheaded by Prof. Stuart Batten and Dr Helen Maynard-Casely and aimed to engage the broader community in the wonders of crystallography. Over 480 Bragg Your Pattern delegates were in attendance over both days. The event consisted of seven awesome activities (based around the seven crystal systems) to inspire the next generation of scientists and ignite a passion for crystallography in young minds, along with an exhibition of patterned artwork, crystallographic-themed fashion, and some gigantic crystal structure models. The activities ranged from helping to build a giant diamond structure (cubic) through to meeting real-life crystallographers (triclinic). Some amazing local volunteers helped, with support from the Cambridge Crystallographic Data Centre, Protein

Data Bank, and the Australian Nuclear Science and Technology Organisation. On Saturday, Prof. Jenny Martin gave a public lecture entitled “How I Fell in Love with Crystallography and why you should too,” which touched upon the history and practice of crystallography, crystallography-themed cakes and the discipline’s enormous impact on science and the world around us.

The completed diamond structure. (Photo credit Chris Sumby)

A particular personal highlight of the Crystal-A-Con activities was the building of a large model of diamond to break the record for the largest chemical model. Over many days preceding the event, the team (mostly at the Australian Synchrotron and including the control room staff) built components of the model, which were then pieced together and extended during the IUCr Exhibition and Crystal-A-Con event. After some stressful hours late on Saturday, when the team thought they were going to be ejected before the model was completed, the final layers were added, and a few defects were removed with minutes to spare. The final numbers, courtesy of Prof. Stuart Batten, were 62,356 atoms + 121,547 bonds = 183,903 parts or 341 kg, with dimensions over the 24 layers being a bottom edge of 3.69 m, top edge of 2.31 m and height of 1.11 m.

To celebrate the 75th anniversary of the IUCr, a dedicated microsymposium, the IUCr 75th Anniversary was held on the afternoon of the second to last day of the Congress. This touched upon topics ranging from the role and importance of the IUCr in international science, to what the various committees and instruments of the organisation do, through to opportunities for the future of the society. These latter points focussed on making sure everyone feels welcome in crystallography and looking to future applications of the science and technique. Reflective of some these ideals, the 26th IUCr Congress had childcare available throughout the entirety of the meeting and had 16 registered children in attendance.

The IUCr Congress dinner, themed as a “Night at the Museum” Congress Celebration Party was held at the Melbourne Museum on Monday night. The Congress dinner was included into all registrations to make it inclusive. Guests were welcome to explore many parts of the Museum, seeing the exhibits and sampling food from Melbourne, Victoria, and Australia. Some fantastic images of people mixing under dinosaur skeletons and being photographed with performers dressed as giraffes, geishas, and Egyptian cats marked this a night to remember for all who attended. The dinner certainly provided an iconic location and allowed the attendees to unwind, share experiences, and celebrate the meeting.

An image from the Congress dinner at the Melbourne Museum. (Photo credit 26th IUCr Congress, SDP Media)

The next day after the dinner, delegates were back to hear from the third plenary of the meeting, Prof. Mark Spackman from the University of Western Australia, talking about “Molecules as Crystals”. This was the opening to another full day of scientific activity before the meeting close in the afternoon. The poster sessions, this time on the balcony areas outside the session rooms, were again in full swing on Monday and Tuesday as the second tranche of posters were on display; organised together in this way, it was apparent how many posters were being presented at the Congress. Late on Tuesday afternoon, the 26th IUCr Congress was closed by the Congress Chair, Prof. Michael Parker, bringing to an end a week (and a bit!) filled with scientific exploration and discussion. The closing session acknowledged the dedication and passion of the crystallography community, especially the local organising committee and the international program committee, in bringing the meeting to fruition and looked ahead to future congresses and continued success for the IUCr.

# CRYSTALS HUMANIZED

*Istvan Hargittai and Magdolna Hargittai*

We have collected a few textual and pictorial expressions that refer to crystals anthropomorphically [1]. We dedicate this contribution to Alan L. Mackay on his 97th birthday. Alan has broadened our worldview of structures.

The Czech writer Karel Čapek (1890–1938) wrote about crystals following his visit to the mineral collection of the British Museum. To express his humility in front of these miracles of nature, he added a drawing to his description [2]

Karel Čapek's drawing after his visit to the mineral collection of the British Museum [2]

... But I must speak again about crystals, shapes, colours. There are crystals as huge as the colonnade of a cathedral, soft as mold, prickly as thorns; pure, azure, green, like nothing else in the world, fiery black; mathematically exact, complete, like constructions by crazy, capricious scientists, or reminiscent of the liver, the heart ... There are crystal grottos, monstrous bubbles of mineral mass, there is fermentation, fusion, growth of minerals, architecture, and engineering art ... Even in human life, there is a hidden force towards crystallization. Egypt crystallizes in pyramids and obelisks, Greece in columns; the Middle Ages in vials; London in grubby cubes ... Like secret mathematical flashes of lightning, the countless laws of construction penetrate the matter. To equal nature, it is necessary to be mathematically and geometrically exact. Number and phantasy, law and abundance - these are the living, creative strengths of nature; not to sit under a green tree but to create crystals and to form ideas, that is what it means to be at one with nature!

Aleksandr I. Kitaigorodsky (1914–1985) liked to ascribe crystals anthropomorphic traits. He said when asked about his most important achievement in science: "I have shown that the molecule is a body. One can take it, one can hit with it; it has mass, volume, form, hardness. I followed the ideas of Democritus." [3] Another version of this notion, attributed to Kitaigorodsky that we heard repeatedly, reads: "The molecule also has a body; when it's hit, the molecule feels hurt all over." For Kitaigorodsky this implied possible structural changes upon the molecules entering the crystal structure. This statement was the more remarkable because it signified a departure from his earlier views about the constancy of molecular shape and geometry regardless of whether the molecule was in the gas phase or in a crystal. One of us remembers a chemistry meeting in what at the time was East Germany—the German Democratic Republic—in some respects more Soviet than even the Soviet Union. There, Kitaigorodsky was quoted as referring to molecules as being free in the gas phase but no longer free in the crystal and that loss of freedom would be causing deformation. Part of the audience took it as a political statement as if reading between the lines, equating the crystalline state with a rigid, regimented political system.

Maurits C. Escher (1898–1972), the Dutch graphic artist whose periodic drawings have been so helpful in discussing space-group symmetries, had romantic notions about crystals. The author Bruno Ernst who wrote a book about Escher's art, quoted him [4]:

Long before there were men on this globe, all the crystals grew within the earth's crust. Then came a day when, for the very first time, a human being perceived one of these glittering fragments of regularity; or maybe he struck against it with his stone ax; it broke away and fell at his feet; then he picked it up and gazed at it lying there in his open hand. And he marveled.

There is something breathtaking about the basic laws of crystals. They are in no sense a discovery of the human mind; they just 'are' - they exist quite independently of us. The most that man can do is to become aware, in a moment of clarity, that they are there, and take cognizance of them.

Alan L. Mackay presented another anthropomorphic view that had its roots in his experience as a crystallographer. He expressed it in a poem [5]:

My molecule is sick,

And I have caught the illness too.

Two atoms have temperatures,  
Which are negative,  
And two are not resolved at all.  
How can I find a cure –  
The R-factor is enormous,  
And direct methods fail me?  
Perhaps it is not my métier,  
To be a structure analyst.

The female poet Anna Wickham (born Edith Alice Mary Harper, 1884–1947) in her poem "The Woman and Her Initiative" contrasted her "colloid" self with her husband's "crystalline" character and the impression is that the latter's demeanor left much to be desired [6]:

Give me a deed, and I will give a quality.  
Compel this colloid with your crystalline.  
Show clear the difference between you and me.  
By some plain symmetry, some clear stated line.  
These bubblings, these half-actions, my revolt from unity.  
Give me a deed, and I will show my quality.

In another poem, "Gift to a Jade," it is unambiguous what she meant by her husband's crystallinity [7]:

For love he offered me his perfect world.  
This world was so constricted and so small,  
It had no loveliness at all,  
And I flung back the silly little ball.  
At that cold moralist I hotly hurled  
His perfect, pure, symmetrical, small world.

Alan L. Mackay has done much to expand crystallography to embrace more among the structures of nature than merely the regular and the periodical. He pioneered handling systems with varying degrees of regularity in their structures, and he wrote about this not only in scientific treatises, but also in his poetry. We quote here an example about flying through the clouds [5]:

We cruise through the hydrosphere,  
Our world is of water, like the sea,  
But the molecules more sparsely spread,  
Not independent, not touching,  
But somewhere in between,  
Clustering, crystallizing, dispersing  
In the delicate balance of radiation  
And the adiabatic lapse rate.

A beautiful example of imbuing crystals with human qualities is in the crystallographer Charles W. Bunn's (1905–1990) drawings [8] and the writer John Ruskin's (1819–1900) words (cited here after [9]):

“Crystal Characters” from Charles W. Bunn's book [8]

And remember, the poor little crystals have to live their lives, and mind their own affairs, in the midst of all this, as best they may. They are wonderfully like human creatures - forget all that is going on if they don't see it, however dreadful; and never think what is to happen tomorrow. They are spiteful or loving, and indolent or painstaking, with no thought whatever of the lava or the flood which may break over them any day; and evaporate them into air-bubbles or wash them into a solution of salts. And you may look at them, once understanding the surrounding conditions of their fate, with an endless interest. You will see crowds of unfortunate little crystals, who have been forced to constitute themselves in a hurry, their dissolving element being fiercely scorched away; you will see them doing their best, bright and numberless, but tiny. Then you will find indulged crystals, who have had centuries to form themselves in, and have changed their mind and ways continually; and have been tired, and taken heart again; and have been sick, and got well again; and thought they would try a different diet, and then thought better of it; and made but a poor use of their advantages, after all.

And sometimes you may see hypocritical crystals taking the shape of others, though they are nothing like in their minds; and vampire crystals eating out the hearts of others; and hermit crab crystals living on the shells of others; and parasite crystals living on the means of others; and courtier crystals glittering in the attendance upon others; and all these, besides the two great companies of war and peace, who ally themselves, resolutely to attack, or resolutely to defend. And for the close, you see the broad shadow and deadly force of inevitable fate, above all this: you see the multitudes of crystals whose time has come; not a set time, as with us, but yet a time, sooner or later, when they all must give up their crystal ghost - when the strength by which they grew, and the breath given them to breathe, pass away from them; and they fail, and are consumed, and vanish away; and another generation is brought to life, framed out of their ashes.

Death is an integral component of life, and the crystalline state is often associated with lifelessness and death. An eloquent description of the beauty and symmetry of snowflakes—water crystals—is given by Thomas Mann (1875–1955) in *The Magic Mountain*. Here, in addition to their breathtaking beauty, Mann expresses also why their high symmetry is associated with a “life-denying character” [10]:

... Indeed, the little soundless flakes were coming down more quickly as he stood. Hans Castorp put out his arm and let some of them to rest on his sleeve; he viewed them with the knowing eye of the nature-lover. They looked mere shapeless morsels; but he had more than once had their like under his good lens and was aware of the exquisite precision of form displayed by these little jewels, insignia, orders, agraffes - no jeweller, however skilled, could do finer, more minute work. Yes, he thought, there was a difference, after all, between this light, soft, white powder he trod with his skis, that weighed down the trees, and covered the open spaces, a difference between it and the sand on the beaches at home, to which he had likened it. For this powder was not made of tiny grains of stone; but of myriads of tiniest drops of water which in freezing had darted together in symmetrical variation - parts, then, of the same inorganic substance, which was the source of protoplasm, of plant life, of the human body. And among these myriads of enchanting little stars, in their hidden splendour that was too small for man's naked eye to see, there was not one like unto another, and endless inventiveness governed the development and unthinkable differentiation of one and the same basic scheme, the equilateral, equiangular hexagon. Yet each, in itself - this was the uncanny, the anti-organic, the life-denying character of them all - each of them was absolutely symmetrical, icily regular in form. They were too regular, as substance adapted to life never was to this degree - the living principle shuddered at this perfect precision, found it deathly, the very marrow of death - Hans Castorp felt he understood now the reason why the builders of antiquity purposely and secretly introduced minute variation from absolute symmetry in their columnar structures.

William Scoresby's sketches of snowflakes from his 1806 logbook after Stamp and Stamp [11]

Snowflake photomicrographs by W. A. Bentley from Bentley and Humphreys [12]

We augment this beautiful prose with the whaling captain and Arctic explorer William Scoresby's (1789–1857) drawings of snowflakes after Tom Stamp and Cordelia Stamp's little-known book [11] and a sample of photographs from W. A. Bentley and W. J. Humphreys' famous book of snowflakes [12]

Scientists have expressed the same, perhaps less eloquently but most succinctly. According to Michael Polanyi (1891–1976) a perfectly ordered environment was not a suitable habitat [13]. The crystallographers Evgraf S. Fedorov (1853–1919) and J. Desmond Bernal (1901–1971) simply stated that “crystallization is death.” [14].

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# THE 50TH ANNIVERSARY OF MACROMOLECULAR CRYOCRYSTALLOGRAPHY

David J Haas

July 1, 2023

Why Macromolecular Cryocrystallography has been so successful

Fifty years after being published, the scientific paper by Purdue Researchers contributed to ending the 2020 Covid-19 Pandemic by quickly providing the three-dimensional structure of the Covid Spike Protein for vaccine development (Structure Guided Drug Design). This research project began in 1965, but the most important phase was performed in the Purdue University laboratory of Michael Rossmann between 1968 and 1969. The results were published in April 1970 (Haas 1970), which described the invention of a means to cryocool protein crystals to near liquid nitrogen temperatures to reduce radiation damage. The paper also described the discovery that cryocooling of protein crystals actually reduced the radiation damage by more than ten times (today, cryocooling is now considered to reduce the radiation damage by more than seventy times (Garman 1997, 2005). Beginning twenty years later, around 1990, cryocooling technology grew into a key element in using Synchrotron radiation for routine X-ray analysis. (The Synchrotron was developed decades earlier but only perfected for protein crystallography after 1970, and produces X-ray beams millions of times greater than conventional X-ray tubes.) Today, with more than fifty Synchrotrons operating worldwide, cryocooling is universally used to reduce X-ray damage during macromolecular crystallography X-ray data collection at every Synchrotron. The Synchrotrons and advanced cryo-cooling have been developed by brilliant scientists, enabling Macromolecular CryoCrystallography to become a routine method of structure determination. In addition, much of the credit for demonstrating the "success of cryocooling" goes to Michael Rossmann, who had the foresight and understanding of its potential! Thank you – once again Michael.

Remarkably, as so often is the case, the "primary" benefits of cryocooling of macromolecular crystals were completely unforeseen by the Purdue scientists.

1 Cryocooling enables repeated X-ray data collection from a single crystal.

2 Cryocooling enables better crystal handling for Synchrotron X-ray analysis and facilitates very rapid data collection with the intense X-ray beam (minutes, not weeks or months).

3 Cryocooling provides a host of operational and molecular/crystallographic benefits for structure interpretation not available at room temperature, such as better stability and easy transport.

Because of the remote access required by the X-ray shielded Synchrotrons, robotic handling is used, and the Synchrotron scientists have provided amazing technology just for this purpose. They are to be congratulated - big-time!

The Personal Story Behind the April 1970 Scientific Paper

With the 1970 published scientific results, I left the field of crystallography to enter industry. In 2004, I had a brief demonstration of cryo-crystallography by Elspeth Garman, but it completely overwhelmed me after 30 years - unfortunately, I did not pursue it. However, in 2015, I attended the ACA Meeting in Philadelphia and then the X-ray Macromolecular Crystallography Course at Cold Spring Harbor Laboratory in 2017, which finally opened my eyes to the subject. I was invited by Stephen Burley to present a seminar at Rutgers PDB on April 24, 2019, and with this preparation, led to the "History of Science" paper published in 2020 detailing this subject (Haas 2020). Surprisingly, I only realized recently that it is the 50th Anniversary of this event. Eureka!

Being able to perform this "proof of principle" research on cryocooling protein crystals in the Rossmann Laboratory was more than just fortuitous. I doubt that I would have been able to perform this experiment anywhere else - one reason is that Michael Rossmann had substantial insight into the future of crystallography, which led him to agree to support the work (and me), and second, the Rossmann Laboratory and Purdue University had all the proper apparatus and personnel that was needed. Hence, I was able to complete the task, which might otherwise have been delayed by years, perhaps decades.

This project began two years earlier (1965) when I arrived for my first Postdoctoral Fellowship position with David C Phillips at the Royal Institution of Great Britain. He had constructed the very first automated X-ray diffractometer, and while collecting data on myoglobin and lysozyme protein crystals a few years before, this radiation damage problem proved to be serious. From this work, he experienced how the X-rays used to analyze the crystals caused them to deteriorate - the same problem that all other protein crystallographers had observed (and lived with!), except with his automatic diffractometer, he could observe the problem in real time (he wrote a scientific paper on this topic: Blake 1962). Therefore, when I arrived, David Phillips suggested that I investigate this radiation damage issue and see if I could reduce the radiation damage. That was the fortuitous beginning of the Radiation Damage Project in September 1965.

I worked on it by myself at the Royal Institution for more than a year without any success. Then during the summer of 1966, David Phillips told me that the crystallographic group was leaving the Royal Institution and that I would need to transfer my work to another laboratory. He had already inquired as to available locations, and the one he suggested was the Weizmann Institute of Science in Rehovot, Israel. My wife Sandra and I agreed, and a few months later, we drove to Israel in late December 1966 with my research supplies in our car, so I could just continue the project there. Little did I know that this was to provide a major breakthrough for the invention of Macromolecular Cryocrystallography?

The Weizmann Institute Crystallography Laboratory was excellent, and the Director, Wolfie Traub provided everything I needed. However, after several more months, I realized that I had to change the direction of the project, so Wolfie and I made a list of possible alternatives. Only one seemed realistic. If I froze (cryocooled) the protein crystals with liquid nitrogen, then this could possibly prevent the X-rays from damaging the protein crystals. In addition, to my surprise, Wolfe had constructed the exact apparatus I needed several years earlier - a liquid nitrogen "gas-jet" cooling apparatus just sitting in the rear of the laboratory - unused. I immediately began the cryocooling experiments.

Within a few weeks I was able to cryocool the lysozyme crystals that I had brought with me. And then when I continued the X-ray exposure for several days to create the radiation damage that I always observed on dozens of crystals, the X-ray diffraction photographs showed little or no changes, indicating possible radiation damage protection. This was the first time I had observed this, and it proved to be a Eureka Moment in my research! I spent the next few weeks performing additional experiments to better understand the phenomena, but this was already May, and the Six-Day War hysteria had already begun in Israel. On May 5, the American Embassy announced that all Americans should leave Israel because, if a war begins, there would be no transportation out. So, that same day May 5, 1967, I drove my wife with our six-month-old son to the airport so they could fly to London to stay with our English friends. At the airport, we booked the next flight, and they were safely away within hours. Without my family and most of the staff and personnel at the Weizmann Institute, this kept me from performing all the experiments I had planned.

However, I continued with some of the work even though I had to collect the liquid-nitrogen supply from the Weizmann Institute Supply Building myself. I was the only person in the entire Chemistry Building, and there was basically no one on campus. I just continued on my own, preparing all my meals and telephoning Sandy every day in London. With the war imminent, the Weizmann Institute basically closed, so any idea of completing the research at the Weizmann Institute was dashed.

The war began on the morning of June 5, but we only saw a few military aircraft overhead that day. Sometime in the morning of this first day, a group of Weizmann security personnel came around and instructed the group that they had assembled as to what we were to do during this time of war. I was told I would be in charge of fire protection for the Stone Administration Building. They showed me where the fire hoses were within the building. In a fifteen-minute training session, I was "fully" trained, more or less, in how I was to fight any fire that should develop and whatever I needed to do if the building was damaged. With my portable radio and a bunch of books, I camped out on the porch of the building, sleeping there for the next three nights. Some of the security staff came by occasionally, but on the third day, they said the war had progressed sufficiently that there was no danger of aircraft, so I could return to my apartment.

The war was over in just six days, but in conversations with the few Weizmann staff that remained, they indicated that the Institute would not be reopened for many months, as everyone would remain in the military forces until the peace negotiations ended. I realized that I would need to make an immediate decision on the matter.

Since I had previously arranged for a position with Michael Rossmann at Purdue University (during my previous year's job search in September 1966), I only needed to check that the position was still available. I contacted Michael to confirm this. He said I could return at any time, as he was certainly aware of the Six-Day War situation. Hence, I decided to return to the United States as soon as possible. This proved a good decision, so I packed all our belongings into our car, said goodbye to several individuals I knew who were still around the Institute, and drove to the Port in Haifa. Remarkably, within minutes, I located a ship sailing directly to London (Tilbury), and so I purchased the ticket, drove to the side of the ship where they loaded our car onto the deck with a crane, and wow - I was in England within days. What luck!

If not for these fortuitous events, the proof experiments of 'reduced radiation damage' by cryo-cooling crystals would probably have been delayed for decades. In addition, my final phase of work with Michael Rossmann would probably not have occurred elsewhere as Michael was only convinced by the "perfect" lysozyme X-ray precession photographs from the Weizmann Institute. He quizzed me extensively and studied all the precession photographs as if it were my final exam. Still, I was sure that the work at Purdue would provide quantitative evidence (proof) for reduced radiation damage. And that is precisely how it happened!

The Rossmann laboratory was a state-of-the-art crystallography laboratory and there were a host of postdocs and graduate students: Margaret Adams, Alan Wonacott, Michael Schevits and Alex McPherson. They were all working on the lactate dehydrogenase protein (LDH) project (Wonacott 1968). The laboratory was very pleasant, and the group was always willing to help me learn the new methods. I had written a short paper describing my Weizmann Institute findings for reduced radiation damage at -50C on the return trip to the United States, so this was distributed to Michael and the other members of the Rossmann group for their support of my project proposal (Haas 1968).

Everyone was certainly skeptical of the benefits of possibly extending the useful life of the crystals, but I was adamant that it was worthwhile even though the 'perceived' complexity and difficulty of building, installing and operating cryo-apparatus may be a barrier. I think everyone assumed that the radiation-damage reduction would be only a few hours, certainly not the hundreds of hours that resulted. (No one could even imagine the importance of cryo-cooling crystals with synchrotron-radiation sources.) Again, the only convincing demonstrations of reduced radiation damage were the lysozyme precession photographs from the Weizmann Institute, but the general notion at the time was that cooling protein crystals would damage them to a point where the X-ray data could not be collected.

After weeks of discussion, Michael agreed to loan me one of the Picker automated X-ray diffractometers for three months (and no more!) in the spring of 1968, and he would fund the purchase and construction of the most primitive cryo-cooling apparatus if I put the system together myself. (It probably would only be used once for my project anyway.) The Purdue Supply Department arranged for liquid nitrogen to be delivered and provided me with several large Dewar Flasks. The Purdue glass workshop fabricated a coaxial gas-delivery jet for directing the nitrogen gas onto the crystal with a dry-air outer barrier jet surrounding the nitrogen stream. I made it to exactly match the Weizmann Institute apparatus. Initially, the single crystals were each mounted in a Lindemann glass vial in the conventional manner along with a small amount of mother liquor exactly as had been done for more than thirty years, but soon after that, I froze the crystals positioned near the end of a single glass fiber where it remained attached by a small amount of frozen liquid. This was a major step forward. Michael wanted the work to be performed on his protein (lactate dehydrogenase, not lysozyme), and enough of his crystals were available for me to use (this proved to be an important decision!). Sucrose was tested as a cryoprotectant to prevent ice formation in the lactate dehydrogenase crystals as soon as the cryo-equipment was ready - it worked perfectly.

A temporary setup was rigged up for the precession camera, which successfully obtained precession photographs of cryo-cooled LDH crystals. Therefore, after Michael approved the project in late 1967, the

cryo-apparatus was ready to perform the data collection in the spring of 1968. The Purdue Glass Making Facility and Laboratory Supply group were invaluable. With the cryo-gas tube assembly ready, simple control circuits were fabricated, and we purchased a suitable air dryer and several bathroom scales for tracking the weight of the liquid-nitrogen-filled Dewars (the scale weight indicates the remaining liquid nitrogen in the Dewar). Three months of work were required for the data-collection portion of the project, and I began the work in April 1968.

We found that initially cooling the protein crystals in a cold gas jet was unsuitable because the crystal faces nearest the gas jet froze more rapidly and asymmetrically. Thus, the usual mounting procedure consisted of placing a single LDH crystal (approximately 0.5 mm of each edge) on a strip of filter paper with a dropper to remove excess liquid, scooping the crystal up on the end of a 0.25 mm diameter glass fiber, and immediately plunging it into liquid nitrogen. The crystal was instantly frozen isotropically to the glass fiber and immobile. As the glass fiber tip had previously been mounted and aligned to the center of the goniometer head, the crystal was also nearly centered for the diffractometer. Finally, the fiber with the protein crystal was transferred quickly from the Dewar full of liquid nitrogen to the diffractometer, where a streaming jet of cold nitrogen gas prevented thawing. Ice formation was prevented by using a coaxial dry nitrogen jet around the cold jet and by surrounding the whole diffractometer with a polyethylene bag filled with dry-nitrogen gas. A statement in our 1970 paper says that a thermocouple placed near the end of the cold jet provided a (nearly) continuous record of the crystal temperature, approximately -75 degrees C.

The data collection proceeded from the first day, with only a few interruptions when mechanical issues with the Picker diffractometer occurred. We also collected data from LDH crystals at room temperature to prepare a comparison graph of a radiation-damage reference reflection (showing data collected at both 273C vs -70C). Punched cards controlled the Picker diffractometer, and it was run 24 hours a day with only a few delays. Otherwise, I fell into a routine for several months of loading the punched cards, filling the Dewar flask with liquid nitrogen, and regularly checking the intensities of the two reference reflections to ensure that the crystal was aligned correctly. The experiment continued unimpeded for three months - this was a very exciting time.

We processed the data during the late summer and fall of 1968, and Michael spent several months analyzing the electron-density maps from our collected data (Haas & Rossmann 1970). The data produced nice results, with the most important graph from these experiments showing a comparison of the reduced X-ray spot intensity decay of the two reference reflections. This radiation-decay graph (Figure 3; Haas 2020) indicated that the X-ray damage in cryo-cooled LDH crystals was reduced more than tenfold at -75 degrees C compared with room temperature data. It was the first quantitative measure of radiation-damage reduction (finally, quantitatively proof!). Michael wrote the final draft of the paper and submitted it to *Acta Crystallographica* in July 1969. The tenfold reduction was low compared to the seventy-fold number that is now accepted, probably because of the higher temperature and temperature variations due to the nitrogen gas jet on the crystals. Reduced radiation damage on cryo-cooling crystals was independently confirmed by Gregory Petsko in his 1975 study on protein crystals at subzero temperatures (Petsko 1975). This certainly contributed to the recognition of the benefits of cryocooling.

In 1969, after interviewing for positions at several universities and pharmaceutical companies, a perfect industrial position became available. I left Basic Scientific Research in 1970 and joined the electronics industry as an X-ray scientist in May 1970 (Philips Electronic Instruments in Mount Vernon, New York), ending my protein crystallography career. I regret not being more diligent with my brief encounter in 2004 at the Chicago ACA meeting and in Oxford with Elspeth Garman and Louise Johnson, but finally, in 2015 when at lunch with Fran and Alex McPherson, he explained to me that cryocooling of protein crystals had become a universal technology for X-ray Synchrotron data collection. He said it was used at all fifty Synchrotrons around the world and used regularly by all protein crystallographers. I was amazed! I have now concluded that in 1970 I had so rejected and repressed any thoughts of cryocrystallography that this explains why I was totally unaware of the subject for 30 years.

Cryo-cooling was slow to be implemented, even though several crystallographers experimented in the field between 1975 and 1990. After 1970, it appears that crystallographers generally knew the benefits of cryocooling. After 1995, most protein crystal structure data were collected at synchrotrons with their crystals

being cryocooled. (This is because the Synchrotrons produce X-ray beams millions of times more intense than the older conventional vacuum X-ray tubes and destroy the protein crystals within seconds.) In addition, the development of Structure-Guided Drug Design became widely used (see review Goodford, 1984) and was developed rapidly during the early 1980s. Structure-Guided Drug Design has been a motivating force for the pharmaceutical industry, and with the AIDS epidemic in the 1980s, protein crystallography, synchrotrons and cryo-cooling had already become a major force for attacking these issues.

In early 2017, I was fortunate to be invited to attend the Cold Spring Harbor X-Ray Macromolecular Crystallography Course, which had been given for more than two decades. In addition to this being my first direct exposure to modern crystallography after more than forty-five years, I was able to participate in laboratory work employing cryocrystallography. I never thought much about this until I began reading about the 'AIDS Lazarus Effect' (Cold Spring Harbor Laboratory 2016). The AIDS Lazarus effect is just one example of the successes of Structural Biology. Later that year, on being invited by Stephen Burley to give the weekly Rutgers Protein Data Bank Seminar on April 24 2019, I reviewed the extensive literature regarding the history and chronology of macromolecular cryo-crystallography. For more than thirty years, synchrotrons have been successfully used for the X-ray data collection on thousands of protein crystals. This is clearly demonstrated by the fact that more than 94% of all FDA-approved drugs used PDB protein structures employing cryocooling (see the Garman figure in Haas 2020). The cryocooling invention developed and demonstrated in the Rossmann Laboratory at Purdue University has proven itself in real-world drug design and as one of the main technologies of the Structural and Molecular Biology fields today. Furthermore, personally, my life is being extended because of one of these pharmaceuticals - Eureka!

I cannot thank enough the many scientists and groups who have enabled me to fill in this fifty-year knowledge gap, and in particular, Elspeth Garman, whom I am privileged to know.

Note: Photo taken 2018 at Brookhaven National Laboratory Synchrotron, Radiation Damage Conference

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## Sparking Interest in STEM: The National Crystal Growing Competition in Canada

*Michelle Dao, Joy-Lynn Kobti, and V. Nicholas Vukotic*

The Chemical Institute of Canada (CIC), a non-profit association of professionals in the chemical sciences, hosts outreach events every year across the country, such as the National Crystal Growing Competition. The goal of the competition is to promote chemistry, chemical engineering, and chemical technology to the youth and to inspire the next generation of scientists and crystallographers through an exciting, educational, and interactive competition. The National Crystal Growing competition has been active for over thirty years. This occurs every fall semester and is open to almost all students, including those who are home-schooled plus teaching staff. Individuals or teams can enter the competition whose aim is to grow the largest and highest-quality crystal possible. The task at hand can be challenging, as many factors affect the crystal growing process (i.e., temperature, vibrations, etc.), which will likely result in students performing trial and error to succeed. This allows the students to develop critical problem-solving skills and to have basic laboratory experience by using various equipment and glassware. After a few weeks of waiting, the crystals are then submitted and evaluated on a regional, provincial, and national level. Students and their teachers can win various prizes ranging from textbooks and swag to cash prizes, with the first prize historically being ~\$350 cash.

The 2022 winning crystals of copper(II) sulfate pentahydrate.

Last year, in 2022, many schools participated across Canada. The 2022 winners for best overall crystals were Rebecca Rouhana, Paulina Abou-Nehme and Zackary Hamwi from Collège Catholique Samuel-Genest (Ottawa, ON). The runner-ups for second and third place were Mathis Poirier-Larouche from École d'éducation internationale de Laval (Laval, QC) and Samuel Giguère from École secondaire Veilleux (St-Joseph-de-Beauce, QC), respectfully. The 2022 winners for the highest quality crystals are Tyeson Bergen, Owen Flaming, and Kailee Tait from Leamington District Secondary School (Leamington, ON). The 2nd place and 3rd place winners are Amélia Barriault and Tina Scherrer from École Monseigneur-Labrie (Havre St-Pierre, QC), and Heather Tocher and Selina Liu, Fleetwood Park Secondary (Surrey, BC), respectfully.

The competition has resulted in various high-school and university news stories, which showcase the dedicated outreach efforts of the regional coordinators across Canada. These include highlights from schools such as Polyvalente des Abenakis, The Conseil des écoles catholiques du Centre-Est, the University of Waterloo, and the University of Windsor. A science department head at the Catholic Central High School in Windsor, Ontario notes, "During COVID time, when there was limited availability of extracurricular activities, this competition gave some of my chem students a great opportunity to do something exciting and fun." Windsor regional coordinator and professor from the University of Windsor, Nick Vukotic, says it was fun to be part of the event, and he looks forward to doing it again and highlights that "it is a great way to get students involved in chemistry and excited about science in general."

Another high-school teacher from the Laval School of International Education also shared that the "competition is very educational for someone who loves science and intends to pursue this field further. Crystal growth is a long-term endeavor that requires precision, patience, and perseverance. Choosing the right "crystal seed," nurturing its growth, and regularly changing the growth solution—these tasks all take time and develop essential qualities for any aspiring scientist."

Kailee Tait, Tyson Bergen, and Owenn Flaming are 10th graders at Leamington District Secondary School who won the Best Quality award at Canada's 2022 National Crystal Growing Competition (left image). Jessica

Fisher, Damien Sharpley, and Jasmine Vo are from Jacob Hespeler Secondary School and were part of a group of students who came in tenth at the National Crystal Growing competition in 2012.

The CIC's National Crystal Growing Competition is an engaging event that promotes chemistry to students and the public, sparking interest in STEM. By taking part in STEM outreach, we can play a pivotal role in shaping young minds, fostering curiosity, and making a lasting impact. Participation and support are not only welcomed but actively encouraged. For more information about how to get involved in the Canadian competition, check out <https://www.cheminst.ca/discover/national-crystal-growing-competition/>. Readers are invited to immerse themselves in the exciting realm of STEM outreach, embracing opportunities such as the National Crystal Growing Competition.

## 2022 U. S. Crystal Growing Competition

*Jason Benedict*

"We really appreciate the contest and prizes. My students love growing crystals, some of them even got kits so that they can grow crystals at home. Thanks so much" –Haley Metcalf, 6th grade Science Teacher at Franklin Park Middle School in Salem, IL.

2022 was another great year for the US Crystal Growing Competition (USCGC, Figure 1, <http://www.uscrystalgrowingcompetition.org/>)! Once again, thousands of kids, parents, and educators from all over the country participated in the #2022USCGC! None of this would be possible without the tremendous efforts of the USCGC Crystallites: Fernando Uribe-Romo (University of Central Florida, UCF), Michael Nippe (Texas A&M University, TAMU), Karah Knope (Georgetown University, GU), Tasha Benedict (University at Buffalo, UB), and Jeffery Rack (University of New Mexico, UNM)! A HUGE thank you to all of their wonderful students, and mine too who helped make the #2022USCGC happen!

The 2022 USCGC began during National Chemistry Week in mid-October and concluded in early December. Hundreds of kilograms of alum went out, and over 160 crystals were sent to UB for judging – a new record!!! (Figure 2) For an awesome photo-essay of the judging, check out: <https://ubuffalo.exposure.co/the-challenge-of-crystal-growing>

There was an exciting addition to the line up of 2022 judges this year! Two local educators and USCGC participants joined the panel: Dana Pepe (Olmstead School #64) and Jeff Yap (Williamsville South High School). It was so fun and rewarding to help get educators more involved in the contest! As judges, they had the opportunity to see all of the submissions firsthand and take new ideas and the experience back to their classrooms!

Holding the judging back at UB (Figure 3) meant a return for many veteran judges including Andrea Markelz (UB, Physics), David Lacy (UB, Chemistry), Travis Nelson (UB, Geology), Luis Velarde (UB, Chemistry), Jeff Rack (UNM, Chemistry). But we were certainly happy to welcome many new judges too: Luis De Jesus-Baez (UB, Chemistry), Andrew Murkin (UB, Chemistry). And lastly, we were so glad that Jacob Furst (UCF), a graduate student in the lab of Fernando Uribe-Romo, made the trip to judge!

"Thanks so much again. Students love participating in this kind of active hands-on learning and it lets me teach them not only about the crystallization process, but also about science concepts like controlling variables, solubility, impurities, chemical sedimentary rocks and cave formations." – Haley Metcalf, educator at Franklin Park Middle School

Winners once again came from across the country! For grades K-8, the Derby North Middle School Science Club with students in grades 6-8 led by Kimberly Norden won both 1st place overall (\$200), and 1st place highest quality crystal (\$100)! Zacia Emniser, Hunter Williams, Shanelle Pruden, and Teagan Lobek, a team of 6th graders from Mrs. Haley Metcalf's class at Franklin Park Middle School (Salem, IL), won 2nd place Overall (\$100, Figure 4). And Charles Rambo, a 5th grader from the Geauga Engineering and Robotics 4-H club in Novelty, OH took home 3rd place Overall (\$50).

"The kids absolutely love this contest. Every year. Every kid. Thank you so much for all the time and energy you put into it. It is so fun to do with them." – Lucy Walter, educator at Lyme/Old Lyme High School

In the 9-12 grade division we also had another dual category winner from the same school - Susan Schmidt's class at Somerville High School in Somerville, MA!! 1st prize Overall (\$200) went to a team of 10th graders Jameer Perez Sinclair, Camden Pereira, and Brian Rodriguez (\$200, Figure 5) and 1st place Highest Quality crystal (\$100) went to Sebastian Ungar. Chase Calderon, Eli Goldberg, and Andrew (Quinn) Sprankle, 10th graders from Lucy Walter's class at Lyme/Old Lyme High School in Old Lyme, CT won 2nd place Overall (\$100, Figure 6). Lucas Watts, Daniel Armendariz-Huang, and Ayomi Odetoyinbo, 10th and 11th graders from Jim Burdick's class at HC Williams High School in Canton, NY won 3rd place Overall (\$50, Figure 7).

"Every year, my students say that growing crystals was one of their favorite activities of the year. I connect it to ionic bonding and how the arrangement of ions affects the properties and shape of the macroscopic crystal. Thanks for running this contest every year - my students are thrilled to have won 1st place. You have helped spark interest in chemistry, and I hope more and more schools participate each year!" – Susan Schmidt, educator at Somerville High School in Somerville, MA.

"The contest gives me a bit of a mission to focus on in the fall before each week starts getting interrupted with delays and snow days. Very excited we finally cracked the top 3!" – Jim Burdick, educator at HC Williams High School in Canton, NY.

The 'Best Teacher Crystal' was won by Karen Metcalf from Cornerstone Learning Community in Tallahassee, FL. Coolest Crystal? This year there were 40 submissions to this category! With so many submissions and growth in this category, we may need more than 'coolest'! Once again, a "super dark purple – nearly black crystal" won!!!! It was sent in by Kate Bryson and Gavin Michaels, 8th graders from Mrs. Lisa Matejka's class at Trinity Lutheran School in Bloomington, IL. I've said it before, and I'll say it again. I never tire of seeing what happens when kids and their imaginations combine with crystals (Figure 8)!!!

"It just grew this way. I have never done this before, and it is awesome!" - Ke'asia Thompson from Margaret Beeks Elementary (Blacksburg, VA) assisted by Elizabeth Larsen (Margaret Beeks) and Amanda Morris (Virginia Tech).

All of the winners were once again announced Academy Award Style on TikTok:

K-8: <https://www.tiktok.com/@uscrystalcomp/video/7192622823288868142>

9-12: <https://www.tiktok.com/@uscrystalcomp/video/7192626792765607211>

Teacher: <https://www.tiktok.com/@uscrystalcomp/video/7192627430119591211>

Coolest: <https://www.tiktok.com/@uscrystalcomp/video/7192643357506555179>

Please check out all the winners and some great participant posts on the contest website and at #2022USCGC on Twitter!

The USCGC helps raise public awareness of the importance of crystal-based research and the organizations, including the ACA, that promote and support these important activities. The USCGC gratefully acknowledges the support of our sponsors: ACA, National Science Foundation, Ward's Scientific/VWR, Pritzker School of Engineering at the University of Chicago, Bruker AXS, Rigaku, Krackeler Scientific, Cambridge Structural Data Centre, the Western New York section of the American Chemical Society, the Departments of Chemistry of UB, GW, UCF, UNM, and TAMU. Please consider making a tax-free donation to the 2023 contest! For more information, please visit the USCGC website or e-mail Jason Benedict at [jbb6@buffalo.edu](mailto:jbb6@buffalo.edu).

Jason Benedict

Figure 1: Hand of Travis Nelson examining a submission during judging of the 2022 USCGC. Photo credit: University at Buffalo | Meredith Forrest Kulwicki

Figure 2: Entries from the 2022 USCGC on display in the Department of Chemistry at the University at Buffalo. Photo Credit: Jason Benedict

Figure 3: Lots of judges hard at work scoring the entries for the 2022 USCGC. Photo credit: Meredith Forrest Kulwicki

Figure 4: Hunter and Zacia (back) and Teagan and Shanelle (front) winners of 2nd place Overall for grades K-8 from Franklin Park Middle School (Salem, IL). Photo credit: Haley Metcalf

Figure 5: (Left to right) Camden, Jameer, Brian, and their teacher Susan Schmidt, winners of 1st place Overall for grades 9-12 from Somerville High School (Somerville, MA).

Figure 6: (Left to right) Eli, Quinn, and Chase, winners of 2nd place Overall for grades 9-12, from Lyme/Old Lyme High School (Old Lyme, CT). Photo credit: Lucy Walter

Figure 7: (Left to right) Daniel, Ayomi, and Lucas, winners of 3rd place Overall for grades 9-12 from HC Williams High School (Canton, NY). Photo credit: Jim Burdick

Figure 8: Top ten "Coolest Crystals" for 2022 viewed in white light (upper) and black light (lower). (1) "super dark purple – nearly black crystal" sent in by Kate and Gavin from Mrs. Lisa Matejka's class at Trinity Lutheran School in Bloomington, IL. Photo credit: Jason Benedict

## **AICS2023 – Pisa 3 – 6 July 2023**

*Annalisa Guerri and Paolo Pio Mazzeo*

**ELECTRON CRYSTALLOGRAPHY:** A deep dive into nanocrystals

The annual school of the Italian Crystallographic Association was held in Pisa from the 3rd to 6th of July. The Organizing Committee, all members belonging to the University of Pisa (Marco Taddei, Enrico Mugnaioli, Francesca Nerli, Giulio Bresciani, Gabriele Paoli, Michele Alderighi) selected 34 students from 9 different EU countries (Denmark (4), Austria (1), Poland (1), Sweden (1), Slovenia (1), Spain (1)), and 4 from non – EU countries (UK (2), India (2)).

The program of the school was organized with theoretical lessons and practical sessions so that students could learn the basis of the electron diffraction theory and then apply it during the workshops which involved the use of different software packages (SIR2019, SHELX, PETS, JANA and OLEX2).

During the school a get together dinner was organized at the beginning of the event to allow people to get to know each other and a social dinner close to the end of the course.

All the students were satisfied with the concept learnt during the school.

## **Summer School on Mathematical Crystallography, Nancy, France, 12-16 June 2023**

*Massimo Nespolo*

The fifth edition of the Summer School on Mathematical Crystallography in Nancy was held last June on the campus of the Faculty of Sciences and Technologies of the Université de Lorraine. It welcomed 28 participants (16 males, 12 females) from 19 countries and 4 continents, representing 26 institutions from 13 countries and 4 continents. Lodging and restoration were provided on-site.

The program included group theory, exercises on the International Tables for Crystallography and on the Bilbao Crystallographic Server, as well tutorials on the Jana2020 software package. The lecturers were Prof. Massimo Nespolo (Université de Lorraine), Prof. Mois Ilia Aroyo (Universidad del País Vasco, Bilbao, editor of Volume A of the International Tables for Crystallography), Dr. Michal Dušek (Czech Academy of Sciences) and Dr. Andrey Zameshin (Malvern Panalytical), supported by Dr. Isabella Pignatelli (Université de Lorraine) as tutor. Poster presentations from the participants were on display during the five days of the school.

The school benefited from the generous financial support of the International Union of Crystallography, the European Crystallographic Association, the Association Française de Cristallographie, the Société Française de Minéralogie et Cristallographie, the Université de Lorraine (via the Doctoral School of Chemistry, Materials and Physics and the Pôle scientifique CPM), the Grand Nancy Metropolitan Government, and Malvern Panalytical as industrial partner. More than half of the budget was used to help students and young scientists to attend the school by partially covering their expenses.

This school was organized in the framework of the activities of the IUCr Commission on Mathematical and Theoretical Crystallography, which had been slowed down by the SARS-CoV2 outbreak.

Details on the school and the list of participants can be found on the school website  
<https://www.crystallography.fr/mathcryst/nancy2023.php>

## 72nd Annual Denver X-ray Conference Report

*Stephanie Jennings*

ICDD, Newtown Square, PA

Format, Dates & Attendance

The 72nd Annual Conference on Applications of X-ray Analysis, more commonly known as the Denver X-ray Conference or DXC, was held 7 - 11 August 2023. The week-long conference returned to the Chicago area, visiting The Westin Chicago Lombard, Lombard, Illinois, USA. X-ray and materials scientists gathered at the conference to discuss various techniques, applications, software, instruments, and products for XRD and XRF analysis. The combination of attendees and exhibitors brought the attendance to over 375 X-ray scientists, with over 30% from outside the United States.

DXC Workshops

The technical program began with 16 half-day tutorial workshops held on Monday and Tuesday of conference week. Topics were categorized as either XRD, XRF, or Special Topic and focused on both beginner and advanced levels. 45 specialists were invited to participate as workshop instructors, and many provided handouts that were posted on a private website for attendees only. Topics included:

What the APS Upgrade will bring to X-ray Analysis – Parts I & II

Cultural Heritage

Basic to Intermediate XRD

Basic XRF

In situ Battery Measurements

Quantitative XRF

Sample Preparation for XRF

Intro to GSAS-II

Advanced Topics in GSAS-II

Texture

Micro XRF

XRF of Layered Structures

XRD Methods for Complex Multi-Phase Identification

How to Get the Best from Your Handheld XRF Spectrometer

## XRF Trace Analysis

### Plenary Session and DXC Awards

The Plenary Session, Energy Storage, was held on Wednesday morning as the opening session for the oral talks that were presented during the next three days of conference week. Scott Misture, Alfred University, chaired the plenary, which began with an awards presentation.

The Barrett Award, given biennially to recognize outstanding contributions to the field of powder diffraction, was presented to Ashfia Huq of Sandia National Laboratories, USA. Dr. Huq received the award for her commitment to and leadership in the advancement of spallation neutron powder diffraction and for her service to the neutron powder diffraction community.

Figure 1 (L-R) Barrett Award Winner Ashfia Huq of Sandia National Laboratories, USA, pictured with Conal Murray, IBM T.J. Watson Research Center, Yorktown Heights, USA.

The Jenkins Award, given biennially to recognize scientists who exhibit lifetime achievement in the advancement of the use of X-rays in materials analysis, was presented to Tim Elam of the University of Washington, USA. Dr. Elam received the award for his contributions to X-ray fluorescence spectrometry in the development of instrumentation and methods of X-ray analyses in challenging environments, including the PIXL micro-XRF spectrometer on the Mars rover Perseverance. The award also recognized his many contributions to educating and teaching others in the field of X-ray spectroscopy.

Figure 2 (L-R) Jenkins Award Winner Tim Elam of University of Washington, USA, pictured with Tim Fawcett, ICDD, Newtown Square, USA.

Also presented during the DXC Plenary Session was the 2022 ICDD Hanawalt Award, recognizing distinguished, recent work in the field of powder diffraction. The Hanawalt Award was presented to Karena Chapman of Stony Brook University, USA. Dr. Chapman received the award for her contributions to developing X-ray diffraction capabilities in the study of challenging materials problems in sustainable energy and environmental remediation.

Figure 3(L-R) Hanawalt Award Winner Karena Chapman of Stony Brook University, USA, pictured with Tom Blanton, ICDD, Newtown Square, USA.

Eight outstanding young scientists received the 2023 Robert L. Snyder Student Grant Award. The awardees and the works they presented at the conference were:

Dana Alramahi, Illinois Institute of Technology, USA, High Entropy Oxide Tungsten Bronzes as Anodes for Lithium Ion Batteries, XRD Poster Session

Karen Castañeda Marin, Illinois Institute of Technology, USA, United Kingdom, Synthesis and Characterization of MoP Nanoparticles Used As a Catalyst in CO<sub>2</sub> Reduction Reaction, XRF Poster Session

Sven Hampel, Clausthal University of Technology, Germany, Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods, XRF Poster Session & Investigation of the Genesis of Spinel Solid Solutions in Recycling Slags, Energy Storage and Harvesting Session & Determination of Diffusion Coefficients of Vanadium Inside Polymer Electrolyte Membranes, General XRF Session

Benjamin Hulbert, University of Illinois at Urbana Champaign, USA, Specimen Displacement Correction for Powder X-ray Diffraction in Debye-Scherrer Geometry with a Flat Area Detector, General XRD Session & Crystal Structure Solution and Thermal Expansions of CaZr<sub>4</sub>(PO<sub>4</sub>)<sub>6</sub> and SrZr<sub>4</sub>(PO<sub>4</sub>)<sub>6</sub>, XRD Poster Session

Hao Lin, Illinois Institute of Technology, USA, Exploring the Structural Evolution in Li-Rich Layered Materials via Operando XRD, XRD Poster Session

Benard Lawer Patawah, Illinois Institute of Technology, USA, XAS Study Local Atomic Environment Mn-Edge in MnOxGO Nanocomposites as Air-Cathode for Metal-Air Battery Application, XRF Poster Session

Himihami Mudiyanse Senevirathna, Illinois Institute of Technology, USA, In Situ EXAFS Study on Pd @ Ni(OH)<sub>2</sub> during Electrocatalytic CO<sub>2</sub> Reduction Reaction, XRF Poster Session

Philipp Ziegler, TU Wien, Austria, Tackling Low Z Element Quantification with TXRF, XRF Poster Session

Figure 4 2023 Robert L. Snyder Student Grant Award Winners.

Following the awards presentation, the plenary session continued with three fascinating talks by keynote speakers Y. Shirley Meng, Argonne National Laboratory, USA, Karena Chapman, Stony Brook University, USA, and Will Chueh, Stanford University, USA. Dr. Meng presented the talk, Designing Better Materials for Future Batteries. Next was Dr. Chapman's presentation on X-ray Visions: Operando Insights into Functional Energy Materials. Lastly, Dr. Chueh presented on Dynamic Electrochemical Phenomena at the Mesoscale. The session was very well attended and offered great insight into future advancements in science and technology.

Figure 5 2023 Plenary Speakers (L-R) – Karena Chapman, Y. Shirley Meng, Scott Misture (Session Chair), and Will Chueh.

### Special Sessions

From Wednesday afternoon through Friday morning, 16 half-day oral sessions were held. Over 100 presentations were organized in the oral sessions, with 30 presentations given by invited speakers, experts in their respective fields. Topics included:

#### New Developments in XRD & XRF Instrumentation

Imaging

Stress and Texture Analysis

Trace Analysis

Machine Learning Techniques in X-ray Analysis – Parts I & II

Synchrotron Applications in XRD

Industrial Applications of XRD

General XRF

Industrial Applications of XRF

General XRD

Quantitative Analysis of XRF

Energy Storage and Harvesting

Cultural Heritage

Applications of Rietveld Analysis

Micro XRF and Synchrotron Applications

#### Poster Sessions

Posters were presented on Monday and Tuesday evenings during the XRD and XRF poster sessions. Two E-poster stations were also set up in the exhibit hall. Attendees were given the opportunity to preview electronic copies of the posters at the E-poster stations or through the mobile app, Whova. Respected judges chose the best posters, and the competition was strong.

Ultimately, the following presenters were named winners:

#### XRD Best Poster Awards:

James Kaduk\*, T. Ens, N. Boaz, North Central College, USA

T. Blanton, A. Dosen, ICDD, USA, for their work:

Crystal Structures of Large-Volume Commercial Pharmaceuticals

Benjamin S. Hulbert\*, J.E. Brodecki, W.M. Kriven, University of Illinois at Urbana-Champaign, USA, for their work:

Crystal Structure Solution and Thermal Expansions of  $\text{CaZr}_4(\text{PO}_4)_6$  and  $\text{SrZr}_4(\text{PO}_4)_6$

Dana Alramahi\*, O. Marques, C. Segre, Illinois Institute of Technology, USA, for their work:

High Entropy Oxide Tungsten Bronzes as Anodes for Lithium Ion Batteries

Figure 6 XRD Poster Session Award Winners (L-R) – Ercan Cakmak (Poster Judge), James Kaduk, Dana Alramahi, Benjamin S. Hulbert, and Tom Watkins (Poster Judge).

XRF Best Poster Awards:

Ruthmara Corzo\*, NIST, USA

J. Stallworth, T. Gluodenis, Lincoln University, USA, for their work:

Elemental Characterization of 3D-printed Polymers Using Micro X-ray Fluorescence Spectrometry for Forensic Applications

Sven Hampel\*, F. Sand, U.E.A. Fittschen, Clausthal University of Technology, Germany

G. Peponi, Fondazione Bruno Kessler, Italy, for their work:

Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods

Karen A. Castañeda\*, I. Senevirathna, C. Segre, M. Asadi, Illinois Institute of Technology, USA, for their work:

Synthesis and Characterization of MoP Nanoparticles Used as a Catalyst in  $\text{CO}_2$  Reduction Reaction

Figure 7 XRF Poster Session Award Winners (L-R) – Ruthmara Corzo, Karen A. Castañeda, Diane Eichert (Poster Judge), Sven Hampel, Maggi Loubser (Poster Judge), and Poulami Dutta (Poster Judge).

We would like to thank two of our exhibitors for sponsoring additional Best Poster Awards during the XRF Poster Session, Amptek, Inc. and XOS.

Amptek Award for Best Student XRF Poster:

Alyssa Tovar\*, M. Schmeling, Loyola University Chicago, USA, for their work:

Environmental Sampling of Chicago Industrial Corridors

XOS Innovation Award™:

1st Place:

Donald Windover\*, NIST, USA

K.J. Kim, KRISS, Korea, for their work:

Thickness Monitoring Using X-ray Fluorescence in Hafnia Films

Runner Up:

Sven Hampel\*, F. Sand, U.E.A. Fittschen, Clausthal University of Technology, Germany

G. Peponi, Fondazione Bruno Kessler, Italy, for their work:

Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods

Exhibits and Sponsorships

The exhibition hall accommodated 36 companies with displays of products and services for the X-ray community. See a complete listing of exhibitors and their product descriptions in the 2023 Onsite Program at [www.dxcicdd.com](http://www.dxcicdd.com). The Denver X-ray Conference is very appreciative of their support this year.

Many of the exhibitors also supported the conference as sponsors, including Amptek, Inc., Anton Paar, Bruker, ICDD, KETEK GmbH, Materials Data, Petrick GmbH, Rigaku Americas, Xenocs, and XOS. The generosity of our sponsors helps to keep attendee costs low and the quality of the conference high. We are grateful for their support!

### Website and Proceedings

To view the complete DXC Program, please visit the 'Past DXC' page of the conference website, located under the 'About DXC' tab at [www.dxcicdd.com](http://www.dxcicdd.com). The conference proceedings, *Advances in X-ray Analysis*, Volume 67, will be published in the summer of 2024. Select papers will also be published in the *Powder Diffraction Journal*. Please also visit the 'Resources' tab on the ICDD website [www.icdd.com](http://www.icdd.com), for free full access to manuscripts published in Volumes 40 through 66 of *Advances in X-ray Analysis*.

The Conference Services team at ICDD would like to thank the many people who volunteered their time and efforts to organize this event. Members of the DXC Organizing Committee, Session Chairs, Workshop Instructors, Invited and Contributed Speakers, and Exhibitors all played a role in bringing the community together again. Special thanks also to the attendees who joined us as well. The success of the event is attributed to each and every individual who participated, and we send our genuine thanks to all of you!

### 2024 Meeting

Save the date! In 2024, DXC will return to Colorado, 5-9 August, at The Westin Westminster, Westminster, Colorado, USA.

## HATFEST!

*Marjorie Senechal*

Figure 1. Craig Kaplan's animation of the Hat family (for the link and details, see [3]).

This summer's Hatfest at Oxford University was a seamless hybrid of conference and festival. For two joyous days (July 20 and 21), we celebrated the Hat, while papers were presented, arguments percolated, and research plans were laid.

Figure 2. Participants in the Oxford Hatfest creating a tiling with paper hats. (Photograph by Stan Sherer.)

Figure 3. The red paper hats in Figure 1 are mirror images of the white hats.

Just four months before, David Smith, a retired printer and tiling hobbyist in Yorkshire, UK; Joseph Myers, a combinatorics specialist in Cambridge, UK, Craig Kaplan, a computer scientist at the University of Waterloo in Canada, and Chaim Goodman-Straus, a tiling theory expert at the Museum of Mathematics in New York, had posted a jointly authored, 89-page, preprint, "An Aperiodic Monotile" [1], on [arxiv.org](https://arxiv.org). The Hat, as the tile was dubbed, made world headlines at the speed of light.

The search for a single shape that tiles the plane, but never periodically, goes back to the early 1970s, when Sir Roger Penrose's tilings by kites and darts showed that "order" and "translation" aren't synonyms. And if two shapes can tile aperiodically, what about one? Several monotile candidates were proposed over the ensuing years whose features (periodic layers, discontinuities) prompted mutterings: that's not what we were looking for! But now here's the Hat, a simple thirteen-sided polygon nestling in a periodic tiling of the plane (Figure 3).

Figure 4. (Fig 1.1 of [1]) A small portion of an infinite Hat tiling.

David Smith (Figure 5) discovered the Hat while "messing about" with the PolyForm Puzzle Solver app [2].

Figure 5. David Smith at the Hatfest. Photo by Stan Sherer

He knew that an aperiodic monotile was a tiling holy grail and as the regions he tiled grew larger and larger with no translations in sight, he thought he might have found one. He contacted Kaplan, who contacted Myers and Goodman-Strauss. Together, the quartet proved that

- a) the Hat is indeed a tile (its copies fill the plane without gaps or overlaps);
- b) all Hat tilings are nonperiodic (they proved this in two very different ways);
- c) the Hat is just one of an infinite family of aperiodic monotiles obtained from it by increasing or decreasing the lengths of its edges (see Figure 1 and [3]).

Moreover, in those four months between the posting and the Hatfest, other scholars showed that Hat tilings are aperiodic crystals (i.e., their diffraction patterns consist of sharp Bragg peaks), that the diffraction patterns have six-fold rotational symmetry (Figure 6), and that Hat tilings can be generated by cut-and-project methods like those used for Penrose and other aperiodic tilings [4].

Figure 6. Diffraction pattern of a Hat tiling (Socolar, [4].)

Still, some muttered that that's not what we were looking for! Hat tilings include -- and must include -- both the hat and its mirror image, but those are two different tiles! Or are they? Euclid considered them to be the same, and so does the authoritative *Tilings and Patterns* [5]. Objection overruled! Nevertheless, the four authors quickly tweaked a member of the Hat family into an aperiodic monotile (which they called a spectre) that tiles the plane without its mirror image [6].

The Hatfest was organized by four British scientists: Felix Flicker (physics, Cardiff University), Nick Jones (Oxford Mathematical Institute), Henna Koivusalo (mathematics, University of Bristol) and Mike Whittaker (mathematics, University of Glasgow). Fittingly, it was held in Oxford's Mathematical Institute, whose splendid courtyard is paved with a Penrose tiling (Figure 7).

Figure 7. Entrance to the Andrew Wiles Building, home of The Mathematical Institute at the University of Oxford. Photograph by Alain Goriely, 2013. (Creative Commons Attribution-Share Alike 3.0)

The unprecedented excitement over the Hat is due to its remarkable properties, the internet, and the generosity of the authors, who freely shared their ideas and software. And also to its accessibility from several vantage points. As everyone at the Hatfest could attest, understanding the Hat draws on the full discovery-justification spectrum, from hands-on "messaging about" to case-by-case computation to hefty theory. Everyone could, and did, jump right in.

The first day of the festival was designed for the broadest of audiences. Natalie Frank (Vassar College) brought the audience up to speed on the math. Sir Roger Penrose (University of Oxford) described the development of his two aperiodic tiles and asked whether there might be a completely different type of aperiodic monotile, one that's not situated in a periodic tiling. In my talk, I showed how paradigms baked into tiling theory and crystallography over the centuries had ingrained the periodicity paradigm. Craig Kaplan told the inside story of the discovery of the quartet's collaboration. There were hands-on workshops, too. David Smith and Jean-Marc Castera led one on the Hat, and Lorenzo Sadun (University of Texas) led another on origami. Hatfest participants assembled a Hat tiling (Figure 1) during a reception and discussion with artists. The first day concluded with a public lecture by Chaim Goodman-Strauss and a panel discussion with the day's speakers, chaired by Henna Koivusalo. At one point, I think during Chaim's talk, Felix Flicker told me later, "I looked back over the full lecture theatre (we had around 330 people signed up in the end) and saw people from all walks of life delighted to be hearing about this fascinating discovery. One person was wearing a Hat hat, while another was wearing a Hat dress. People were drinking Hat beer. Outside the theatre, the walls were lined with Hat artwork, including a hand-sewn quilt that had taken thousands of hours to make. People are thrilled about it in a way I haven't seen before for other discoveries."

Talks on the second day -- see [7] for the full list of speakers, affiliations, lecture titles, and abstracts -- situated the Hat in up-to-the-minute tiling theory and in the growing field of aperiodic order. And Adolfo Grushin (CNRS, Grenoble) discussed joint work with Felix Flicker on possible applications in physics and materials science, in which they found that Hat tilings sit "in a previously unoccupied place in crystallography between quasicrystals and crystals." And, looking at the behavior of electrons in tight binding models based on the Hat, they found properties remarkably similar to the 2D-periodic crystal, graphene. (Other properties lie closer to models of disordered materials and quasicrystals.)

The Hatfest was the second meeting of the Grimm Network [8], founded by the four organizers to honor the memory of the mathematician and physicist Uwe Grimm (Open University, UK), who died unexpectedly in 2021. "Uwe was always really welcoming, bringing together as broad a range of people as possible to create an international community interested in aperiodic tilings," Felix Flicker explained. "We sought to continue his legacy by bringing together mathematicians, physicists, artists, hobbyists, and more. I think Uwe would have been very proud of the event and his legacy."

I am pleased to dedicate this note to Uwe, who was my colleague and friend. I hope that future meetings of the Grimm Network will keep us up to date on this rapidly burgeoning field.

## References

- [1] David Smith, Joseph Samuel Myers, Craig S. Kaplan, Chaim Goodman-Strauss, An aperiodic monotile, arXiv:2303.10798, v1 submitted 19 March, 2023.
- [2] <https://www.jaapsch.net/puzzles/polysolver.htm>
- [3] <https://cs.uwaterloo.ca/~csk/hat/>
- [4] Joshua E. S. Socolar, Quasicrystalline structure of the Smith monotile tilings, arXiv:2305.01174, v1 submitted 1 May 2023. (See also Michael Baake, Franz Gähler, Lorenzo Sadun, Dynamics and topology of the Hat family of tilings, arXiv:2305.05639, v1 submitted 9 May 2023. )
- [5] Branko Grünbaum and Geoffrey Shephard, Tilings and Patterns, W. H. Freeman and Co., 1987.
- [6] David Smith, Joseph Samuel Myers, Craig S. Kaplan, Chaim Goodman-Strauss, A chiral aperiodic monotile, arXiv:2305.17743, 28 May, 2023.
- [7] <https://sites.google.com/view/thegrimmnetwork/hatfest>

## ICCGE20

*Annalisa Guerri*

International Conference on Crystal Growth and Epitaxy

Naples 30 July – 4 August 2023

The 20th edition of the International Conference of Crystal Growth and Epitaxy was held in Naples at the University Campus of S. Giovanni a Teduccio.

The Conference should have been held in 2022 following the schedule of the 3 years between one conference to the other but due to the pandemic, it has been postponed to 2023.

The participants were almost 600 coming from 40 different countries and the presence of female participants was around 35%. Also, the attendance of the students was significant. All the scientific sessions were all well populated.

At the end of the conference, several prizes were awarded: the Frank prize was appointed to Peter Vekilov, University of Houston (USA) and Juan Manuel Garcia-Ruiz, Instituto Andaluz de Ciencias de la Tierra (Spain), for significant fundamental contributions to the field of crystal growth, the Laudise prize to Peter Rudolph, Crystal Technology Consulting (Germany), for significant technological contributions to the field of crystal growth and the Schieber prize was awarded to Bharat Jalan, University of Minnesota (USA) to recognize the outstanding value of his scientific publications in the field of crystal growth.

Finally, the Rostislav Kaishev was awarded for best oral presentation by young scientist to Isha Bade, Imperial College London (UK) and Artur Tuktamyshev, University of Milano Bicocca (Italy).

Photo\_IUCr\_grants: Awardees of the IUCr grants, from left to right Arnab Kar, IIS, Bangalore (IN), Durgesh Singh Sisodiy, HBNI, Mumbai (IN), Adhikari Abinash, Polish Academy of Science, Warsaw, (PL), Annalisa Guerri LOC, Veronika Grigoreva, RAS, Novosibirsk (RU), Hanna Dabkovska, IUCr President, Charlotte

Vernozy-Trouillet, École Polytechnique, Paris (FR) and Andrea Zappettini, Conference Chair. Missing: Ekaterina Kochetkova, Leibniz Institute for Solid State Research Dresden (DE) and Nerith Rocio Elejalde-Cadena, Institute of Physics UNAM, Mexico City (MX).

## Crystallographic Reflections: A History of the Society of Crystallographers in Australia and New Zealand

*Roderick J Hill*

I joined the (then) Society of Crystallographers in Australia (SCA) soon after its formation in 1976 and was privileged to serve as its Honorary Secretary for three terms from 1982. However, work eventually took me away from direct participation in crystallographic research, and I lost touch with the Society. Many years later, after reconnecting, I realized that crystallography and the Society had changed significantly. The original pioneers of the Society, to whom it owed a great debt, were greatly diminished in number, and unless its rich and illustrious history was soon recorded, it would be lost forever. In early 2022, I contacted the then President (Megan Maher) and the Council of the now Society of Crystallographers in Australia and New Zealand and offered to write its history. To my delight, they accepted my offer; some snippets from the resultant manuscript are provided below.

.....

The Society of Crystallographers in Australia and New Zealand (SCANZ) has existed in three configurations over the last 60+ years. The first version is generally recognized as emerging in May 1961 in association with the first 'open' (i.e., not just internal institutional) meeting of Australian crystallographers (since dubbed 'Crystal 1') at the University of Sydney. This meeting of what later became known as the 'Bush Crystallographers' was the initiative of Hans Freeman, then Professor of Chemistry at the University of Sydney. Hans was also central to the movement in 1973 to establish the Society of Crystallographers in Australia (SCA) and was elected as its inaugural president at the Crystal 10 meeting in Richmond, NSW, in April 1976. In acknowledgment of the major and long-term engagement of colleagues from 'across the ditch' (aka New Zealand), the name was changed to the Society of Crystallographers in Australia and New Zealand (SCANZ) at the Crystal 21 meeting in Thredbo, NSW in February 2000.

The original Bush Crystallographer 'members' were a small group of individuals who, for the most part, had learned their trade as postgraduate or postdoctoral students overseas, working with some of the icons of crystallography in the early post-WWII period (inter alia, Kathleen Lonsdale, Linus Pauling, Dorothy Hodgkin, Edward W Hughes, and J. Monteath Robertson). Among these, first-generation Australian pioneers in the early 1950s and 1960s may be counted: Hans Freeman (Sydney University), 'Sandy' Mathieson, Barrie Dawson and Dave Wadsley (CSIRO), Jack McConnell and Nev Stephenson (University of NSW), Maureen Mackay (La Trobe University), Alan White, Jim Graham and Ted Maslen (University of Western Australia), Bryan Gatehouse (Monash University) and Terry Sabine (Australian Atomic Energy Commission, now ANSTO).

They established the first tranche of significant crystallography laboratories in Australia and were key players in the organisation of the early Crystal meetings and the formation of the SCA. Their graduate students, in turn, established second-generation groups at other universities and research institutions in Australia and overseas. A corresponding group of New Zealand crystallographers founded major laboratories at Industrial Research Lower Hutt (George Patterson), U Auckland (F.J. Llewellyn), U Canterbury (Bruce Penfold) and U Otago (A.J. Ellis). Figure 1 shows some of these key players at Crystal 1 at Sydney University in 1961, and Figure 2 shows several others, probably at Crystal 4 at Lucas Heights in 1966.

Figure 1. Some of the participants at the first Bush Crystallographers Meeting (Crystal 1), organised by Hans Freeman at Sydney University, 25–26 May 1961. L to R: John E.W.L. Smith, Janet and Max Taylor, Anne and Gordon Robinson and John Cowley, annotated with their (later) SCA connections. Image credit: IUCr photo gallery.

Figure 2. Prominent pioneers of crystallography in Australia, pictured around 1966, perhaps at Crystal 4 at the AAEC, Lucas Heights. L to R: Dave Wadsley, Sandy Mathieson, Janis Friedrichsens, Barry Dawson. Image credit: IUCr photo gallery.

Throughout its existence, both as a collective and through its individual members, SCANZ has played a very significant role in the development of the crystallography landscape in Australia, New Zealand and overseas. It was a foundation partner in the Federation of Scientific and Technological Societies (FASTS), the political lobby group for increased funding for Australian science and technology; it was a major actor in the push for funding for Australian access to major Synchrotron and neutron facilities overseas (the so-called 'suitcase science' / 'Small Country Big Science' initiative). Its members were prime movers in the establishment of the Australian National Beamline Facility (ANBF) at the Tsukuba synchrotron in Japan, and they were also key advocates for the establishment of the Australian Synchrotron and the new OPAL research reactor. They also led or participated in many of the technical committees advising on the type and design of beamlines for those facilities. Along with the Crystallographic Society of Japan, the Society was a strong proponent and prime mover in the establishment of the Asian Crystallographic Association (AsCA) in 1987 and, until recently, one of only four Regional Associates of the International Union of Crystallography (IUCr).

Through the Society's ex officio representative (and other independent members) on the National Committee for Crystallography of the Australian Academy of Science, the Society is (in practical terms) the primary link for Australia's engagement with the IUCr. Society members have acted as President and Vice President of the IUCr, served on its Executive Committee, and occupied seats on all 22 Commissions of the IUCr at one time or another, often as Chair. It has been the organiser of two of the IUCr Congresses and General Assemblies held since 1948, the 14th in Perth in 1987 and the 26th in Melbourne in 2023, and it devoted considerable resources to the Australia-wide celebration of the International Year of Crystallography in 2014. It maintains a strong supportive presence (both financial and participatory) in meetings of AsCA (Asian Crystallographic Association).

Since 1961, its series of regular national meetings (to date, 34 and counting; Figure 3) and, since 1980, its Newsletters (79 and counting) have provided critical and effective platforms for the exchange and dissemination of scientific information, science politics, and personalia, past, present, and future in the domestic and international crystallographic domains.

Figure 3. The approximate locations of all 34 meetings of the Bush Crystallographers, SCA and SCANZ, and the two IUCr Congresses and General Assemblies organised by SCANZ from 1961 to 2023.

The Crystal meetings and newsletters continue to provide an important and fertile connection point for professional and student crystallographers in Australia and New Zealand. They have served to celebrate and encourage the achievements of members and to engender a sense of a crystallographic community across both nations. From interviews with some of the early participants in these meetings (and from my own recollections), they were certainly memorable affairs, often showcasing (aside from science) the musical, singing and raconteurial talents of otherwise quite often shy and retiring scientists. Not to be missed, as evidenced by the small groups of crystallography lecturers from the University of Western Australia and their students who were willing to endure a road trip over 3-4 days (with rotating drivers and sparse accommodation) of more than 3,400 km, in part across the Nullarbor Plain on the then unsealed (dirt) Eyre 'Highway', from Perth to Melbourne to attend the meetings, and back again (Figure 4).

Figure 4. Crossing the Nullarbor Plain from Perth, Western Australia on the 1,700 km long Eyre Highway to attend the Crystal 5 meeting at Monash University, Victoria, in August 1967. L to R: Biswanith Mukajee, Syd Hall, Ted Maslen. Photo credit: Syd Hall, using a time delay on the camera exposure, judging from the shadow of the tripod.

Along with the 'Crystal' and IUCr meetings, SCANZ has organised several significant one-off events, including the Bragg Symposium in Adelaide in 2012 to mark the centenary of the founding of X-ray crystallography by W. Lawrence (born and educated in Adelaide), a field in which he and his father, William H. Bragg made pre-eminent contributions recognised by the award of the Nobel Prize for Physics in 1915. Another event was the 1991 dedication ceremony for the 'A.D. Wadsley X-ray Laboratory', held at the CSIRO Division of Mineral

Products, Port Melbourne, in recognition of his pioneering contributions to crystallography and solid-state chemistry (Figure 5). Participants included David's family and many of his friends and colleagues (most of whom were foundation members of the SCA) from around the country and overseas.

Figure 5. Standing, L to R: David Scaife, Jim Graham, John Watts, Bruce Hyde, Alex Moodie, Jeff Wunderlich, Gus Mumme, Bob Roth, Terry Sabine, Alan Reid, Hans Freeman, Judge Bevan, ??, Sir Alan Walsh, M. Fehlmann, Bryan Gatehouse, ??, Ted Ringwood. Seated: Joy Bear, Sandy Mathieson. Photo credit: Rod Hill.

The structure and culture of the Society have gone through several major changes over its 60+ years. From an ad hoc small informal grouping of most of the early crystallographers in Australia funded by local organising institutions to its present position as a formally incorporated entity with active global engagement, a membership of nearly 300 people, around 50% of whom are students. Its financial resource is now more than AUS\$2.3M, the investment returns from which allow it to offer travel scholarships to prominent overseas speakers and students to attend national and international meetings. These funds also enable awarding of the Bragg and Mathieson Medals to outstanding mature and early-career researchers at each Crystal meeting.

Diversity and gender equity was introduced in 2020 as a formal policy of the Society, applied in particular to Office Bearers and speaking and session-chair roles at all its meetings. It has also instituted a policy of encouraging young researchers through its Rising Stars Awards at each national meeting, along with an allowance for carer's provisions.

From its initial focus (typical of the time) on the crystallography of inorganic materials and minerals, the Society has embraced increasing focus on structural biology as humanity responds to the need for greater understanding of the nature and function of molecules essential to life. It is also adjusting to the massive change in the 'face' of the science of crystallography over the years, from a unique and important discipline in its own right, to a still extremely important, but now largely enabling discipline underpinning the broader biological, materials, chemical and physical sciences. Emerging technologies and software, such as 'cryoEM' and massive protein folding algorithms based on artificial intelligence for the solution of macromolecule structures, are also providing new challenges.

While crystallographic data collection and structure solution is now, for most compounds, largely automated, the need for advances in crystallographic science and equipment to deal with ever larger and more complex materials (especially in the biological domain) has ensured that the discipline remains as important and rewarding for researchers as ever. The Society has greatly assisted adaption to these changes through its generous financial support for student attendance at national and international crystallography meetings and its continued commitment to the teaching of crystallography through its Australian Crystallography Schools (in partnership with the Australian Synchrotron), which have operated since 2008.

As a result of all these actions, the Society's meetings remain relevant and exciting, and continue to attract the best speakers from home and abroad by showcasing the most relevant and exciting science of the day.

Dr Roderick J Hill DSc FTSE FRACI FAusIMM, was Secretary of the SCA 1982-87. He is a former Chief Research Scientist at CSIRO and PVC for Industry Engagement and Commercialisation at Monash University, Victoria, Australia.

## J Bruce Forsyth (1932 – 2023)

*Mike Johnson, Bill David, Andrew Taylor and Jane Brown*

From Mike Johnson, Bill David, Andrew Taylor

Bruce Forsyth was a renowned research scientist who made significant contributions to the study of the atomic structure of magnetic materials through his development of the technique of polarised neutron scattering.

Following a PhD in Cambridge, Bruce moved to Harwell, where he designed and built diffractometers on the Dido and Pluto reactors as part of Harwell's expanding user programme providing access for academic researchers.

He joined the Neutron Beam Research Unit at the Rutherford Appleton Laboratory (RAL) in 1972. The NBRU, under the leadership of Leo Hobbis, had been set up initially to support the development of a research reactor to replace Dido and Pluto. However, with the closure of the NIMROD synchrotron on the RAL site, the opportunity presented itself to build a world-leading pulsed neutron source based on the accelerator infrastructure and expertise at RAL, which eventually became the ISIS Facility.

Bruce played a key role in developing the scientific case for ISIS as secretary of the 'Structure Determination' working group (led by Brian Fender), which assessed the range of science that could be achieved by the new source and outlined the key parameters for a number of crystallographic instruments, including the High-Resolution Powder Diffractometer HRPD and the Single-Crystal Diffractometer SXD.

Promotion to an Individual Merit post soon followed, and Bruce's career developed in instrument building in science and in computing, both at RAL and the Institut-Laue-Langevin (ILL, Grenoble). His computing skills were key to defining the new facility's computing and data acquisition system, and his acronym PuNCH (Pulsed Neutron Computer Hierarchy) lives on at ISIS today. He co-authored the specification-of-requirements document issued to companies bidding to supply the control and analysis computers.

His main scientific contribution was in crystallography, principally magnetic structures, and specifically exploiting the scattering of polarised neutrons, where he made many innovations in tandem with his long-time collaborator, Jane Brown of the ILL. As well as authoring scientific papers on the subject, he was instrumental in producing the Cambridge Crystallographic Subroutine Library CCLS suite of software which is still widely used in the international scientific community.

Bruce retired from RAL in 1997 after 25 years on the international scene but continued to be active with honorary positions at the Clarendon Laboratory, Oxford and the University of Warwick as well as collaborations in Grenoble.

Bruce brought enthusiasm and energy to all his work throughout his career – engaging and positive and always sporting a cravat! He was a 'light touch' manager, allowing and encouraging his team to develop and flourish. He and his wife, Janette, made team members welcome and were generous in making their holiday home in East Portlemouth available to colleagues. Bruce was a class act and a true polymath.

From Jane Brown

Bruce and I first met in 1955 when he joined the alloys group of the Crystallographic Laboratory of the Cavendish Laboratory in Cambridge as a research student. Although Bruce was my elder by a couple of months, he was a year junior in the lab because of the 18 months he spent doing National Service in the RAF. We both worked, under the supervision of Dr. W.H Taylor, on a project sponsored by the American Airforce to study the crystal and electronic structures of aluminium-rich intermetallic compounds. This led to our efforts to determine the electron distributions in these compounds and to the development of one of the very first automatic X-ray diffractometers, 'MAXIM', which received its instructions on punched paper tape from the EDSAC 1 computer.

After completing his Ph.D. in the field of X-ray diffraction, Bruce moved on to Neutron diffraction at the Atomic Energy establishment at Harwell. There he was responsible for building their first (and only) polarised neutron

diffractometer on the Pluto reactor. He was closely involved with the establishment of the University user program at Harwell and finally moved to the Rutherford Appleton laboratory when a Neutron Scattering group to support University users was created there.

When the British joined the ILL associates in 1973, Bruce immediately became involved in the plan to redirect three diffractometers, already ordered for the user program, to the ILL. He had already been planning to upgrade and automate the Pluto polarised neutron diffractometer. He was rapidly able to adapt these plans and propose that they should be used so that one of the three diffractometers should become a polarised neutron instrument. His ideas were accepted, and he became responsible for installing and programming the D3 polarised neutron diffractometer on the H8 beam of the ILL reactor.

He and his family spent the year 1974-75 in Grenoble while the installation was underway. In the following years at RAL, he was a staunch supporter of the UK Neutron scattering program and a frequent visitor to the ILL, where we did many experiments together. Many of these were on D3, but he also exploited several other instruments. Over the years, we developed an increasing interest in the possibilities offered by neutron polarization analysis. After several less-than-satisfactory experiments using conventional techniques, Bruce became a valued collaborator in many of the exploratory experiments to establish methods for carrying out polarization analysis with the zero-field polarimeter Cryopad.

I will remember Bruce as a good friend and close collaborator with a constantly cheerful and outgoing personality.

## **John William White (1937–2023)**

*T.R. Welberry*

Photo published with permission of the Research School of Chemistry, Australian National University, Canberra and David White

John William White AO CMG FRS FAA FAIP FRACI (25 April 1937 - 16 August 2023) was a Professor of Physical and Theoretical Chemistry, Research School of Chemistry at the Australian National University.

It is with sadness that we report that Professor John White, whose name will be familiar to many in Crystallography and Neutron Science circles, passed away at his home in Canberra on 16 August 2023 at the age of 86. Our thoughts are with his wife, Ailsa, his four children and their extended families, and many friends and colleagues. He will be sorely missed by all who knew him.

He was a past president of the Royal Australian Chemical Institute and President of the Australian Institute of Nuclear Science and Engineering. He held the Argonne Fellowship (U. of Chicago) and was for many years a Fellow of St John's College, Oxford. Between 1975 and 1981, he was director of the Institut Laue-Langevin, Grenoble, France. He was a founding member of the International Society for Science and Religion.

John was born and grew up in Newcastle, NSW. He was born on ANZAC day – an important day for all Australians. He was proud of this coincidence and made a point of attending the Anzac Day Parade (held at dawn) whenever he was in Australia. He was the eldest child of George and Jean White and had two younger sisters, Wendy and Gina. Both his parents were immensely supportive and proud of him. He was the first in the family to go to university – at the age of 16. John graduated from the University of Sydney in 1957 with First Class Honours in chemistry and won the Frank Dixon Prize. He went on to obtain his MSc in 1959 and then won a prestigious 1851 Scholarship to continue his studies in Oxford, where he obtained his DPhil and subsequently became a Lecturer and Fellow of St. John's College (at the tender age of 26). He remained in Oxford until 1985, apart from a 5-year period between 1975 and 1981, when he moved with his family to Grenoble to take up the appointment of joint director and then director of the ILL. He returned to Australia in 1985 to take up the appointment of Professor of Physical and Theoretical Chemistry at the Research School of Chemistry (RSC) in the Institute of Advanced Studies at the Australian National University. He maintained his links both with St. John's in Oxford and with the ILL in Grenoble and frequently visited both, usually managing

to do some experiments, either at ILL or at the Rutherford Appleton Laboratory Neutron Source (ISIS) near Oxford. He kept his house in Grenoble.

John was very proud of his association with St. John's College, and it has been said that since that time, the only tie that he ever wore was his St. John's tie. His time in Oxford affected him in many ways, and he valued every moment. His family recalls with affection that he met his wife-to-be, Ailsa, during his early days at Oxford, and he would often relate the story of their first meeting and maintained that it was the single most important and best thing that ever happened in his life. John and Ailsa shared an incredible bond through 57 years of marriage.

Perhaps John's most significant contribution to Australian Science has been his role in getting both the OPAL Neutron Source (in Sydney) and the Australian Synchrotron (in Melbourne) funded by governments and built to the highest international standard. Together, these two research facilities represent at least a \$500M investment in the country's scientific and technological future, and they have accelerated the internationalisation of Australian science, in addition to decelerating the brain drain. While not in the direct management chain, John served on many important committees and used his position in the Australian Academy of Science to help make the political, scientific and business case for both OPAL and the Australian Synchrotron. This has given the next generation of Australian researchers in many fields of science and engineering "the opportunity of a generation" and has allowed them to do their research in Australia rather than to have to travel overseas.

From an early age, John liked to experiment in the laboratory himself. His family recalls that as a schoolboy, he set up a laboratory in his grandmother's house. Every week, he obtained a new chemical from the local pharmacy, on which he experimented using a textbook his father bought him. He claimed never to have had a fire or an explosion! Later, even when he had a large group of students and post-docs working with him, he would still like to be involved himself. He led from the front!

One of the marks of John's career has been the talent that he has nurtured and grown at Oxford and the Australian National University in Canberra, where he has played a leading and influential role for the last 30 years or so. Several of his protégés have become Directors of leading international research centres around the world. The Bragg Institute at the Australian Nuclear Science and Technology Organisation employs at least three of John's students or postdoctoral fellows from the Australian National University. He has deeply influenced the careers of many more.

John was the second President of the Asia-Oceania Neutron Scattering Association and was one of its formation's leading players (along with colleagues in Japan and Korea). As recently as July 2015, he was awarded the AONSA Prize in recognition of his leadership across the Asia-Pacific. He has advised many overseas laboratories, including the CCLRC, in the UK and several others in the USA. Most significantly, he was chair for many years (2002-2012) of the International Advisory Committee for the Japan Proton Accelerator Research Complex, the other leading facility (along with OPAL) of its type in our region.

John has made huge contributions to global science: most notably, I think he must have been the first to open up the new method of neutron scattering (using neutrons from research reactors) to chemistry in the 1960s. This gave British and Australian chemists a leadership position they have never relinquished. In addition, he was a prime mover in using specific deuteration of molecules to change the contrast in such experiments, which now turns out to be the "killer application" of neutron scattering worldwide. Indeed, it was a key factor in Australia's decision in 1997 to build the new OPAL Reactor and later on to fund the world-leading National Deuteration Facility at ANSTO.

Another aspect of John's Legacy to Australia was his involvement in the setting up of the Oxford Australia Scholarship fund over 20 years ago. This Fund was initiated to endow scholarships each year for academically top Australian graduates to go to Oxford University for study and research. John took the lead in raising the endowment, which now totals \$4,500,000, and for those 20 years, he chaired the committee that awards the scholarships annually. So far, about 100 young Australians have benefited from this scheme.

On a personal level, I have enjoyed many stimulating interactions with John, covering a wide range of mutually interesting topics, which I will greatly miss.

## **S. K. Sikka (1942–2023)**

*Nandini Garg*

Dr. S. K. Sikka breathed his last on 21st of June 2023 while visiting his children in Boston. This news not only saddened us high pressure physicists but the entire department of atomic energy India. He was not only an eminent scientist but was also a very wonderful and simple person. He was a great mentor and his enthusiasm even at this age was infectious.

Dr. S.K. Sikka was born on Nov 1942 in city of Jhang of undivided India. After his graduation from Punjab university he joined Bhabha Atomic Research centre (BARC) when he was only 18 yrs of age. He started his scientific career under the mentorship of Dr. R Chidambaram. He held several key positions and went on to become the director of the Atomic and Condensed Matter Physics group at BARC. In 2002, he chose to move to the office of Principal Scientific Advisor to the Government of India as its Scientific Secretary and later became a Homi Bhabha Chair professor.

Dr. Sikka was well known for his pivotal contributions in Pokharan 1 and II. He set up a laboratory with facilities for static pressure generation employing diamond anvil cells and shock waves generation with gas guns, which was the first such laboratory in India. Dr. S. K. Sikka was not only was an ace experimentalist but also an accomplished theoretician.

His early interests were in crystal structure determination of hydrogen bonded materials with neutron diffraction, neutron resonance scattering & neutron anomalous dispersion. His studies of the Phase problem employing anomalous and direct scattering methods have been incorporated in the teaching aids of International Union of Crystallography. One of his significant early studies was on single crystal neutron diffraction studies on potassium oxalate monohydrate at the CIRUS Reactor at Trombay BARC, India. It had been shown that this compound was the only reported structure in which neither of the lone pairs of the hydrogen bonded water molecules was specifically directed despite the availability of metal ions in that structure. In fact the classification of the H-bonded water molecules with respect to their lone-pair coordination, proposed by his team ( J. Chem. Phys. 41, 3616, 1964) is the most extensively used classification in literature. Based on a modified Lippincott – Schroeder potential for the hydrogen bond, he explained why the shorter hydrogen bonds are less bent on the average than the longer ones. His structure solutions on  $\text{Cd}(\text{NO}_3)_2 \cdot 4 \text{D}_2\text{O}$  and  $\text{Sm}(\text{BrO}_3)_3 \cdot 9 \text{H}_2\text{O}$  using anomalous neutron scattering and neutron resonance scattering using two wavelengths were the first reported applications of the use of thermal neutrons in the determination of the phase problem.

Due to his brilliance, Dr Sikka was requested to work in areas, relevant to the departmental programs and thus started working on high pressure behavior of materials. In the initial days the main interest was in the EOS data of materials. Based on the Saha ionization theory, he and his colleagues developed a model to compute the EOS of solids in the intermediate pressure region (500-1000 GPa) (Phys. Rep. 102, 121, 1983). He worked on the high pressure behavior of several actinides. However, apart from this, he also worked on basic research problems in the area of high pressure science. He has a volume of work on the formation of omega phase in alloys and d- rich transition elements under static and shock pressures. His review article ( Progress in Mat. Sci, 27, 245, 1982) on the 'Omega Phase in Materials' is considered to be a textbook by researchers in Condensed Matter Physics/ Materials Science. He worked extensively on high pressure induced crystal to amorphous phase transitions ( Progress in Mat. Sci, 40, 1, 1996). Notable amongst them are his studies on negative thermal materials, quartz like materials and different forms of carbon and silicon.

Dr. Sikka served as a member of the Executive Committee of the International Association for Advancement of Research and Technology under High Pressure, and as a consultant to the Commission on High Pressure of International Union of Crystallography. He chaired the INSA committees for the International Union of Crystallography and Committee on Data for Science and Technology and served as a member of the Asia Pacific Academy of Materials and the editorial board of High Pressure Research journal.

He was the recipient of several awards, notable among them were the H. K. Firodia award for Excellence in Science and Technology, M. M. Chugani Award for Excellence in Applied Physics by the Indian Physics association, and the fourth highest Indian civilian award the Padma Shri. He was the elected fellow of the Indian National Science Academy, Indian academy of sciences and the National Academy of Sciences India.



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