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Contents

Letter from the President

President's Letter – Winter 2023 4

Editorial

Editorial 7

Feature article

John Dalton remembered 10

IUCr activities

The International Tables Symmetry Database – a comprehensive guide 21

IUCr journals news

Acta Cryst. A clocks up 1.25 millionth structure for the CSD 22

Exploring tetrel bonding: a special issue of Acta Cryst. C 23

Editorial

A triumvirate of Section Editors moving Structural Biology Communications ahead 24

Shaping the future of Acta Crystallographica F: unveiling our vision 26

Introduction to the special issue related to the 18th International Small Angle Scattering Conference (SAS2022) 28

Commentary

Electron traps and energy storage: modeling a bright path to the future 31

Mythical compounds 34

Predicting photoactivity in dithienylethene crystalline solids 36

Thinner than a knife's edge: 3D-printed liquid sheet jet technology for solution phase XFEL experiments 40

IUCr Congress

Crystal-a-con at IUCr2023 46

Meeting report (IUCr supported)

73rd Annual Meeting of the ACA: The Structural Science Society (ACA2023) 54

Meeting report

11th Training course on symmetry and group theory 56

Meeting report (IUCr supported)

Electron Crystallography School 2023 59

Meeting report

12th Belgian Crystallography Symposium 67

2023 Meeting of the Crystallographic Society of Japan 69

Notice

CCDC news and updates 73

Obituary

Hendrik (Henk) Schenk (1939–2023) 75

Robert H. Blessing (1941–2023) 77

Press release

Anton Paar looks forward to its 60th anniversary celebrations 80

IUCr supported events

IUCr supported meetings 82

Meetings calendar

Meetings calendar 83

LETTER FROM THE PRESIDENT

President's Letter – Winter 2023



A visit to the IUCr offices in Chester, UK, in November 2023. From left to right: Malcolm Cooper, Alex Stanley, Santiago García-Granda, Trevor Forsyth and Peter Strickland.

Santiago García-Granda

I am writing this letter as we are in the midst of the Christmas season, as we are about to close the year 2023, which marked our 75th anniversary as a scientific organisation, and as we are about to begin 2024.

In the years between IUCr Congresses, 2024 and 2025, the spotlight should be aimed at our Regional Associates, ACA, AfCA, AsCA, ECA and LACA, all of which have announced their next meetings. This will be a wonderful opportunity to take the pulse of the state of crystallography and structural science at a regional level and also to establish new bilateral and multilateral connections between the Regional Associates and the National Committees. The IUCr, through its Meetings Support Committee, is doing its best to facilitate the participation of young scientists and to have the maximum prominence in these meetings and often associated schools. Our journals are very interested in the contributions arising from these meetings.

The calls for nominations for our flagship Ewald, Bragg and Struchkov Prizes are coming soon. The Union makes a significant financial effort to recognise the careers of the most brilliant crystallographers and structural scientists at various stages of their careers, and it is very necessary for us to be able to identify the best candidates in all scientific areas, particularly women. Therefore I ask for your collaboration with the Selection Committees in nominating candidates to ensure that the awardees are the best possible representation of our excellence and our diversity.

The IUCr Committees and Commissions, once consolidated after the renewal of their members approved by the 26th General Assembly in Melbourne, will be renewing their activity in the various scientific and organisational areas that constitute the heart of our Union and that set the guidelines for our future scientific developments. At the moment, all our Commissions are working at a good pace with the autonomy that characterises their mode of operation within the framework of the IUCr, according to the updated guidelines.

Our ten scientific journals and *International Tables*, together with this *Newsletter* and the other IUCr publications, provide the image of both our scientific level and our social contribution. They also provide us with the necessary financial return to maintain our functioning and the patrimony of our activities in order to promote the development of crystallography and structural science in the most economically and academic disadvantaged areas and to ensure the generational renewal of our scientific community.

The new members of the Executive Committee have organised their visits to our office in Chester to familiarise themselves with the activity of the 24 people who constitute the stable nucleus that efficiently carries out our technical and administrative work, essential for the functioning of the IUCr. Also, this group is very conditioned by the inevitable generational handover, for which – under the supervision of our Finance and Executive Committees – the IUCr CEO, Dr Alex Stanley, must plan with a vision for the future.

It was good for the new General Secretary and Treasurer, Professor Trevor Forsyth, and me to meet many of our team in Chester and see the initiatives being implemented to make publishing in our journals more attractive and make our journals more competitive. We also need the help of our scientific Commissions and our Regional Associates and National Committees to convince every scientist to publish their best contributions in IUCr journals. I consider that it is especially important for us to make it easy for young people to make their first scientific contributions to our journals and encourage them to transmit their comments through our *Newsletter* and social networks.

Trevor's role must be decisive in the configuration of the working teams and in the control of the activity of the Chester office and in the control of the finances and resources of the Union. This intention framed our recent working visit to Chester, on 27 and 28 November, where we met with Professor Malcolm Cooper, the Convener of the IUCr Finance Committee, as well as Alex and Peter Strickland, Executive Managing Editor, visiting the different sections of the office and noting the technical and administrative improvements underway, as well as the various threats to the Union.

I would like to remember, emotionally and gratefully, those who left us in 2023 and send a message of appreciation to their families, colleagues and friends. I would also like to welcome those who joined the IUCr, either via their National Committees or as members of the IUCr Associates Programme. I do not want to forget our industrial partners, who are so supportive of our meetings and schools with their financial and technical contributions. Thank you very much for being an important part of the IUCr family.

The process initiated in Melbourne to define our Purpose, Vision and Values in an open and participatory way, to ensure the scientific and social leadership of crystallography and structural science for the remainder of the 21st century, is advancing according to the planned steps. A survey to gather the opinion of the global IUCr community has recently been conducted to concretise the ideas that best define our identity and our objectives. The results will be presented to the entire community once they have been analysed by the Executive Committee.

The Executive Committee, which had its first virtual bimonthly meeting on 7 November and has another planned for 9 January, will meet in person in Denver, CO, USA, in July 2024, coinciding with the ACA's annual meeting. The Finance Committee meeting will be held at the same place in the preceding days. Prior to that, in March, we will have the spring meetings of the Journal Management Board in Chester and the Finance Committee in Lund, Sweden.

The Executive Committee, through its President or some of its members, will try to be present, representing the IUCr, at the most important regional and international events for the IUCr.

Our representative in the International Science Council (ISC), Dr Hanna Dabkowska, has reported on the approval process of the new ISC statutes, which, after intense activity by the International Unions, are proposed with an important protagonism of the International Unions in the decision-making processes of the Organisation. This is good news, which we hope will be confirmed in the coming months. In more good news, I would like to congratulate Hanna on her recent appointment as an ISC Fellow. The ISC Fellowship recognises individuals for their outstanding contributions to the promotion of science as a global public good, and is the highest honour that can be conferred on an individual by the ISC.

The collaborative projects being developed with governments, companies and non-governmental organisations will give an extraordinary boost to the development of science in all regions of the world. The Africa Initiative, led by Professor Claude Lecomte, is achieving important results, and other activities in Kenya, led by Professor JuanMa García-Ruiz, with important local support, are in progress. The

worldwide 2023 IUCr Crystal growing competition for schoolchildren is also in progress. The development of new infrastructures in less developed countries and the project Light Sources for Africa, the Americas, Asia and the Middle East Project (*LAAAMP*) are going well. And the International Year of Basic Sciences for Sustainable Development, now drawing to a close, has served as a prelude to the International Decade of Sciences for Sustainable Development 2024–2032 (IDSSD).

In this time of serious and bloody international conflicts and natural disasters, many of them due to the climate change that our societies are causing, global scientific societies must be able to identify their role in building a better world for future generations, based on scientific, technical and humanistic knowledge. As expressed before, our role is to promote, defend and protect science and scientist, keep ourselves out of fanaticism of any kind, by maintaining 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 open minds, global awareness and the resources and conditions to sustain a better and better life on the planet, and this is not only for the human species but also to maintain the planet's biodiversity and wildlife.

Once again, many thanks to all those who form and make our organisation work, the Regional Associates, the IUCr Commissions and Committees, Editors, Co-editors, referees and authors of our journals, our Chester staff and all individual crystallographers, women and men.

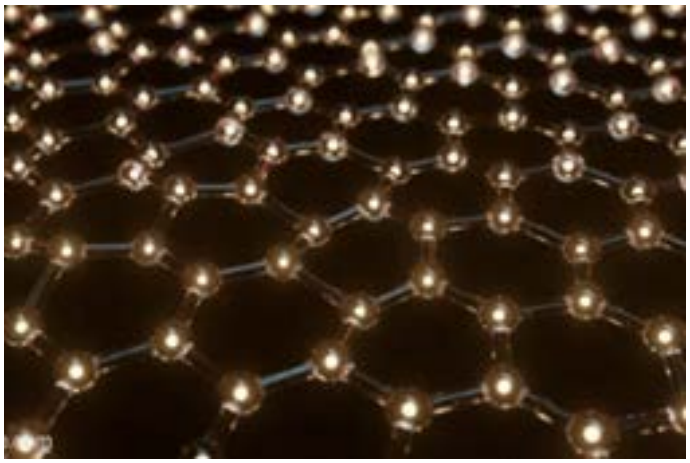
Thanks to *IUCr Newsletter* Editor Mike Glazer, his team and all contributors.

Many thanks to all for keeping the IUCr alive, active, strong and human.

Happy 2024 from all of us!

EDITORIAL

Editorial



Mike Glazer

The IUCr Congress this summer was a great success, with attendees coming from across the world. Bringing schoolchildren into the heart of a scientific congress such as this was brilliant. In this issue of the *IUCr Newsletter*, Stuart Batten, Helen Maynard-Casely, Rosemary Young, Emily Furlong and Bryce Mullens describe this aspect of the IUCr Congress entitled Crystal-a-con. We are indeed fortunate that crystallography and crystal structures can be made to look so attractive and interesting to excite the interest of young people.

The science of crystallography has a long history, but it is only within the last 400 years or so that our understanding of crystals and their atomic structures has "*crystallised*", so to speak. The study of crystallography turns out to have been conducted by many scientists well known for their research into other scientific disciplines. So, for example, Johannes Kepler, famous for his theory of planetary motions, also became interested in the symmetry of snowflakes and also in the close packing of spheres to explain morphology. Then again, Robert Hooke, famous for his Law, among other things, also tried to explain crystal morphology using the packing of spheres (see Fig. 1). So, the principle of periodicity in crystals was the subject of interest for many scientists in the past. One of my scientific heroes, Louis Pasteur, better known for his work on microbes, also started off as a crystallographer with his study of optical activity in tartrate crystals. So, now I see that even John Dalton, whom we all know for his theories on gases and atoms, also had crystallographic leanings. I never knew that, did you? Well, in a feature article, Istvan and Magdolna Hargittai reveal all about this aspect of Dalton's life.

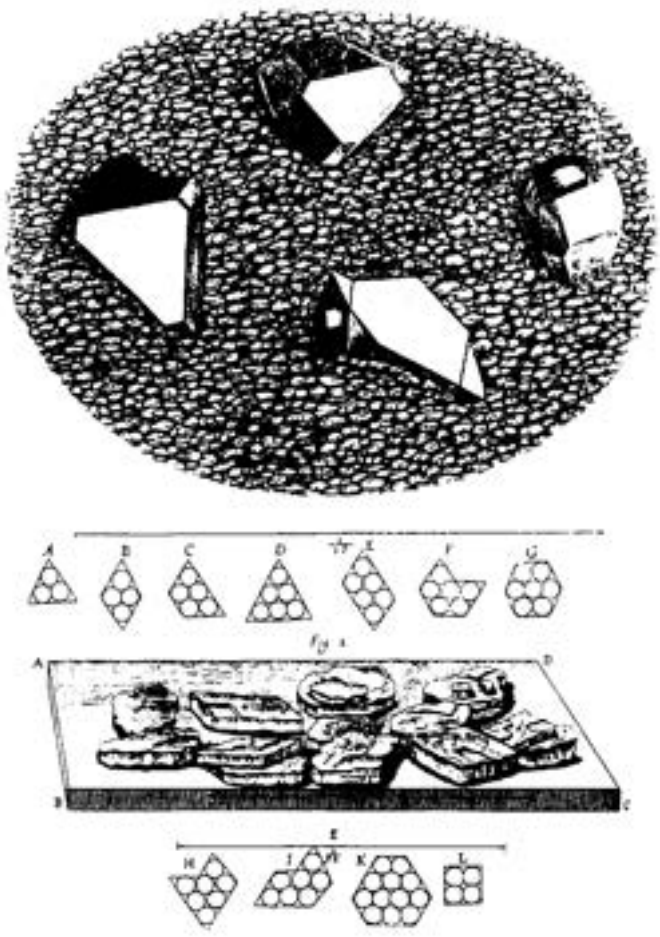


Figure 1. From Robert Hooke's *Micrographia* (1665). The lower diagram is for crystals grown from urine.

One of the problems facing crystallographic publications is how to evaluate the correctness of a particular submitted crystal structure. So, it is incumbent on all referees and journal editors to ensure that at least the proposed structure makes chemical sense. In my experience, there are two or three cases that need attention. Sometimes, it is a matter of fraud. For example, recently, I refereed a paper in which it became evident that the authors had merely copied the coordinates from a much earlier Rietveld refinement published by other scientists and used them with the atom labels changed to match those in their own compound of interest. Then, you have cases of scientific misunderstanding. I am reminded that several years ago, I came close to failing a PhD student during his *viva voce* examination (something that I had never done before) over his quoting of errors in pressure measurements to 7 figures of decimals! Even after explaining that you cannot simply copy out the results of a computer calculation like that, and after he tried to argue that the computer results are correct, he finally agreed to change the errors in his thesis to single figures of decimals, but he did so with exceedingly bad grace. I don’t think he ever really understood my objection despite nearly an hour of trying to explain to him the significance of errors.

The article on mythical compounds highlights problems with structure validation. It is all too easy to collect some data and refine it to apparently good agreement but arrive at a nonsensical crystal structure arrangement. A personal example of this was when I had a paper to referee in which the authors claimed to have carried out a Rietveld refinement on both X-ray and neutron powder data and to have obtained very low, so-called *R* factors. However, they did not give the actual refined atomic coordinates in a table. When they finally revised the paper, I saw that their X-ray and neutron coordinates bore no resemblance to each other. On plotting out their structures, it became obvious that the refined structures made no sense at all! Perhaps an extreme example of mythical compounds has been in the recent publication in *Nature* of the use of generative AI to predict the existence of hundreds and thousands of new crystal structures. Unfortunately, as pointed out in the Twittersphere (or is it X-sphere?) by Robert Palgrave, examination of the structures reveals that many seem to make no chemical sense at all nor provide

powder diffraction patterns that match the experimental measurements! Computers, eh?

Sadly, as usual, we have to report the deaths of two of our distinguished colleagues, Bob Blessing (USA) and Henk Schenk (Netherlands). Both were well known for their scientific research and their services to the crystallography community. I remember many happy discussions with Henk on the crystallography of chocolate, which turns out to be the most essential factor in determining its taste and texture. Crystallography appears everywhere!

FEATURE ARTICLE

John Dalton remembered



John Dalton. © Science Museum Group, used with permission.

Istvan Hargittai, Magdolna Hargittai

John Dalton was a pioneer in modern science. Whenever his name is mentioned, we think of his atomic theory and color blindness ('Daltonism') but seldom of his contribution to crystallography. His ideas about packing in water and in ice were most forward-looking.

When in the years 1983−1985 we were working on our book *Symmetry through the Eyes of a Chemist* in English (its first edition) [1], we found the development of the ideas of dense packing most fascinating. This was something that had hardly interested us before because our principal research was in gas-phase molecular structures where packing was not a subject of consideration. After Lucretius and Johannes Kepler, we enjoyed Dorothy Hodgkin's essay 'Moments of Discovery', referring to the *crystallographer* John Dalton in a collection of papers in *Kristallografiya* honoring Boris K. Vainshtein [2].

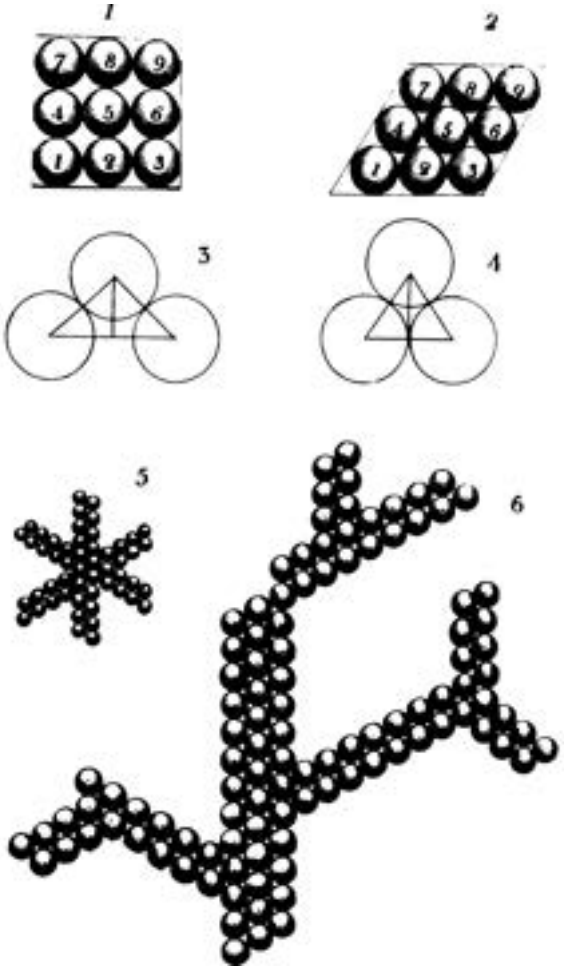


Figure 1. Dalton's models for water (1 and 3) and for ice (2, 4, 5 and 6) in his book *A New System of Chemical Philosophy* ([3], p. 128, plate III).

Hodgkin called attention to the remarkable difference between the packings in liquid water and ice manifested in Dalton’s 1808 treatise (Fig. 1). Dalton's idea was that the building elements in solid ice are more densely packed than in liquid water. Hodgkin showed the reappearance of Dalton’s ideas in the model of the atomic arrangement in the 2Zn–insulin crystal [2]. The molecular structure of insulin is very complicated, but the molecular packing, especially the arrangement of the insulin hexamers, reminded her of Dalton's hexagonal ice.

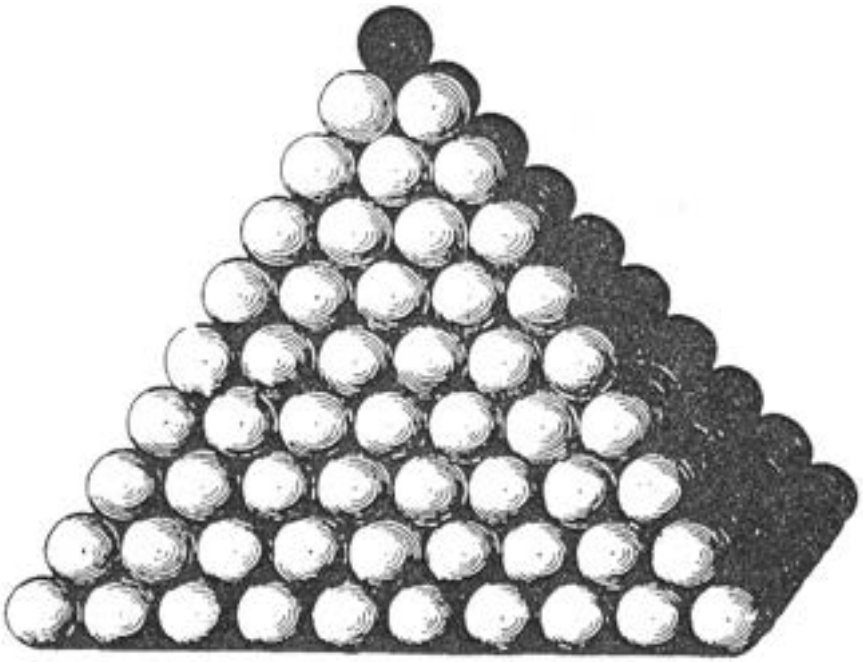


Figure 2. Closely packed spheres by Dalton [4].

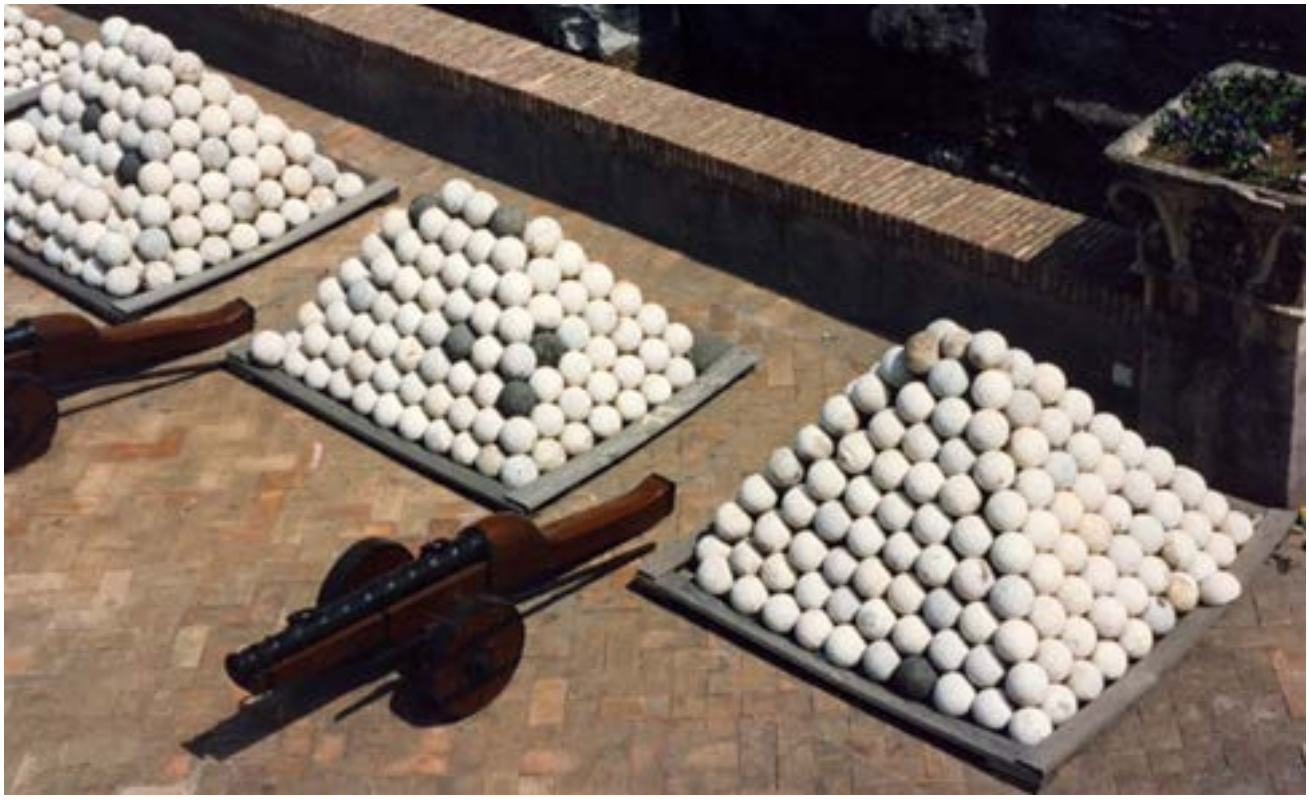


Figure 3. Closely packed cannon balls in the Castel Sant' Angelo, Rome (photograph taken by the authors).

In the third edition of our *Symmetry through the Eyes of a Chemist* [5], we included another representation of the close packing of spheres from John Dalton (Fig. 2) [4] and a photograph of a close-packed arrangement of cannon balls (Fig. 3) ([5], p. 422).



Figure 4. A well-known engraved portrait of John Dalton by W. H. Worthington (1823) after J. Allen (1814) (photograph from the Wellcome Collection).



Figure 5. John Dalton’s mezzotint portrait by C. Turner (1834) after J. Lonsdale (photograph from the Wellcome Collection).

John Dalton’s (1766−1844; Figs. 4 and 5) oeuvre has been treated extensively in the literature and in chemistry texts. We single out the monograph by William C. Henry, which appeared in 1854 and is freely accessible [6]. Following a brief biographical introduction ([7], p. 106), we present a sampler of memorials to John Dalton in the remainder of this communication. It is far from complete and is meant to indicate his international recognition.

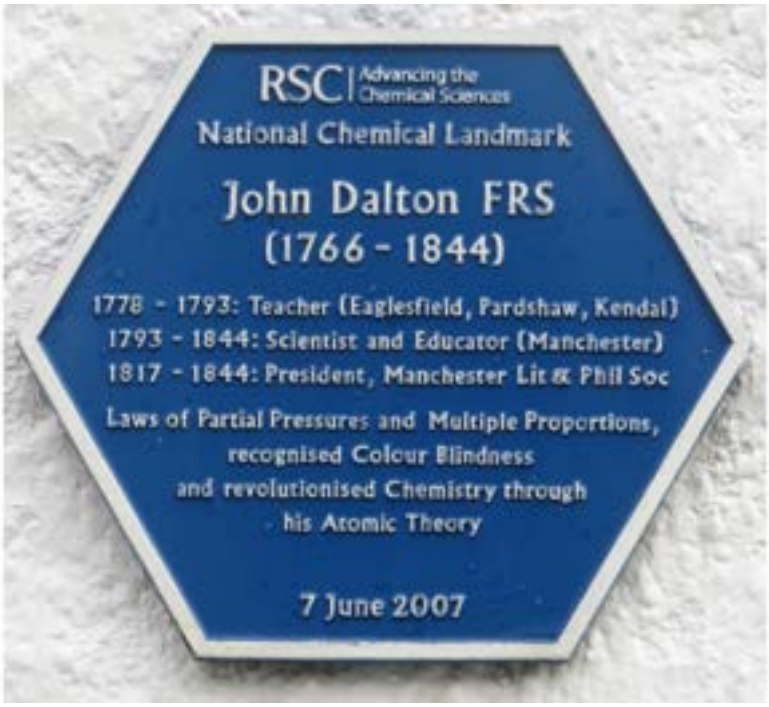


Figure 6. John Dalton's memorial plaque at his birthplace in Eaglesfield (photograph taken by Graham Robson, reproduced under the Creative Commons Attribution-ShareAlike 2.0 license). There is a similar plaque on the wall of the Ape and Apple pub on John Dalton Street in Manchester. Yet another Dalton memorial plaque is on the wall in the offices of the Manchester Literary and Philosophical Society. Dalton was its president from 1816 to 1844.

Dalton was born in Eaglesfield in Cumberland, England (Fig. 6). His parents could not afford to give him a formal education, but he was precocious in self-study, and already at the age of 12, he was teaching at a village school. This was followed by a series of teaching positions and sometimes even school principal positions. He landed a tutorship in mathematics and philosophy in 1793 at the New College of Manchester. It was about this time that he published his first book on meteorology. Other books followed, including one on the familial condition of color blindness, eventually called 'Daltonism'.

He investigated the properties of gases and discovered the Law of Partial Pressures. He is best known for his atomic theory and his charts of atomic weights. He described his theoretical findings in *A New System of Chemical Philosophy,* published in 1808 [2] and appended in 1810. His theoretical discoveries helped the chemical industry establish the correct proportions of the component elements in the compounds being produced.

He was a Quaker, and his modesty made him decline the Fellowship of the Royal Society; although C. Turner's portrait (Fig. 5) says "Dr DALTON, F.R.S.", Dalton accepted an honorary doctorate from Oxford University.



Figure 7. Statue of John Dalton by Francis Chantrey (1838) in Manchester Town Hall (photograph taken by the authors).

It was a great distinction that, in 1838, his statue was created by the distinguished sculptor Francis Chantrey (1781−1841). It now stands in Manchester Town Hall (Fig. 7), opposite James Prescott Joule's (1818−1889) statue by Sir Alfred Gilbert. It is most appropriate to have the memorials of these two giants of science close to each other as the elderly Dalton was a mentor of the young Joule.



Figure 8. Stone portrait of John Dalton on the back façade of the former ICI building, Smith Square, London SW1P (photograph taken by the authors).

Imperial Chemical Industries's (ICI) headquarters was opened in 1929 after ICI was formed from the merger of several companies. ICI left the site in the 1990s following the restructuring of the company giant. Eleven stone portraits of distinguished chemists decorate the façades of the former headquarters. Four of them were directly associated with ICI or its predecessor companies: Harry McGowen, Alfred Nobel, Ludwig Mond and Alfred Mond. The other seven were great contributors to chemistry: Joseph Priestley, Henry Cavendish, Antoine Lavoisier, John Dalton (Fig. 8), Justus von Liebig, Marcellin Berthelot and Dmitri I. Mendeleev. Our guidebook *Science in London* describes the exact location of these stone portraits on the three segments of the façade ([7], pp. 103−110 and 240).

John Dalton's portrait, as an oil painting by Thomas Phillips in 1835, is one of many scientists' portraits in the 300,000-strong collection of the National Portrait Gallery in London, at St Martin's Place, WC2H. The Gallery has been at this location since 1896, but the collection first opened in 1856.



Figure 9. John Dalton as a low-relief statue on one of the six panels on the front façade of the headquarters of the US National Academy of Sciences (photographs taken by the authors).

The United States Congress chartered the National Academy of Sciences of the USA (NAS) as an independent institution in 1863 during the American Civil War. Its headquarters were located for a long time at the Smithsonian Institution. Its current headquarters opened in 1924 at 2101 Constitution Avenue, NW. There are six low-relief bronze panels by the sculptor Lee Lawrie located between the windows on the front façade of the headquarters. Three panels are on the left of the entrance and three are on the right. Each panel depicts six scientists (except the middle right, which depicts seven). John Dalton is on the middle-left panel, which displays the following scientists: Humboldt, Dalton, Lamarck, Watt, Franklin and Huygens (Fig. 9). More about the decorations, including these panels, of the headquarters of NAS can be found in [8].



Figure 10. Two *bas-relief* portraits of John Dalton. Left: on the façade of Olive Tjaden Hall at Cornell University, Ithaca, New York. Right: on the wall of the entrance lobby to the Ceremonial Hall of the tower building, Lomonosov Moscow State University, one among 24 mosaic portraits of Russian and international scientists [9]. Both photographs were taken by the authors.



Figure 11. Two *bas-relief* portraits of John Dalton in Budapest. Left: on the Trefort Campus of Eötvös University, in the building that was first erected for chemistry in 1871. Today, this is part of the Faculty for Humanities ([10], pp. 65−66). Right: on the campus of the Veterinary School ([10], p. 142). Both photographs were taken by the authors.

The above four *bas-relief* portraits (Figs. 10 and 11) expand the international outlook of our collection of Dalton memorials, but should be considered only as accidental examples that must be a small fraction of Dalton memorials worldwide. The present communication also exemplifies that Dalton's legacy belongs to broader domains in science than how his name is usually associated.

We conclude our presentation with an unusual group picture in which Dalton is depicted as one of the central figures in a large group of scientists and technologists.



Figure 12. 'Distinguished British men of science 1807−1808 assembled in the library of the Royal Institution, London. Mezzotint by W. Walker and G. Zobel after F. Skill and W. Walker (*ca* 1860) after Sir J. Gilbert' (photograph from the Wellcome Collection).



Figure 13. A key to the identities of the sitters in Fig. 12 (photograph from the Wellcome Collection).

This image of Fig. 12 has quite some literature (*e.g.* [11] and [12]). There are over 50 men in this image. Careful examination by a science historian has shown that they could never have come together as a group, and the meeting could not have taken place at the Royal Institution. Many distinguished scientists and technologists are in the picture, but many other important scientists are missing, especially in biology, which is hardly represented. The portraits of those presented were copied from other works of art. Thus, Dalton's portrait closely resembles W. H. Worthington's 1823 engraved Dalton portrait (see Fig. 4) with a few minor alterations. The identity of those in Fig. 12 can be determined from the key given in Fig. 13. The period 1807−1808 was George III's reign, who himself was a scientist, although, alas, eventually his mental state prevented continuation of his royal duties. An attractive indication of the popularity of the pioneers of science and technology during the Victorian era was that copies of this group image were available for purchase. Prints of different quality were produced, and they were priced accordingly.

References

[1] Hargittai, I. & Hargittai, M. (1986). *Symmetry through the Eyes of a Chemist*. Weinheim, New York: VCH.

[2] Ходжкин, Д. (1981). *Кристаллография*, **26**, 1029–1045.

[3] Dalton, J. (1808). *A New System of Chemical Philosophy*. Manchester.

[4] Dalton, J. (1805). *Memoirs and Proceedings of the Manchester Literary and Philosophical Society*, Vol. 6, p. 271. Manchester.

[5] Hargittai, I. & Hargittai, M. (2009). *Symmetry through the Eyes of a Chemist*, 3rd ed. Springer.

[6] Henry, W. C. (1854). *Memoirs of the Life and Scientific Researches of John Dalton*. London: Harrison and Sons.

[7] Hargittai, I. & Hargittai, M. (2021). *Science in London: A Guide to Memorials*. Springer Nature.

[8] Hargittai, I. & Hargittai, M. (2023). *Eur. Rev.* **31**, 227–251.

[9] Hargittai, I. & Hargittai, M. (2019). *Science in Moscow: Memorials of a Research Empire*, p. 78. Singapore: World Scientific.

[10] Hargittai, I. & Hargittai, M. (2015). *Budapest Scientific: A Guidebook*. Oxford University Press.

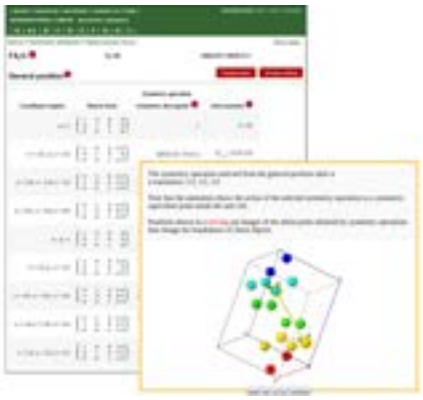
[11] Clow, A. (1956). *Ann. Sci.* **11**, 183–193.

[12] Fara, P. (2001). *Endeavour*, **25**, 91–92.

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IUCR ACTIVITIES

The International Tables Symmetry Database – a comprehensive guide



The *International Tables Symmetry Database*, part of *International Tables for Crystallography*, is a collection of individual databases of crystallographic space-group and point-group information. Programs are provided to access and interactively visualize the data, and also allow new data to be calculated 'on the fly', facilitating the in-depth study of group–subgroup relations, domain structures and twinning, families of related crystal structures and phase transitions, and the prediction of new crystal structures. The *Symmetry Database* has been available since 2011 to subscribers to the online version of *International Tables for Crystallography*, and is periodically supplemented with exciting new features.

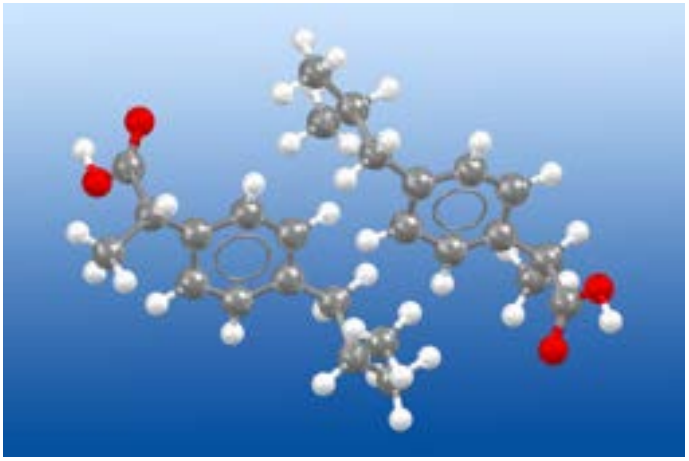
In a highly informative open-access article in the Teaching and Education section of the latest issue of the *Journal of Applied Crystallography*, Gemma de la Flor, Eli Kroumova, Robert M. Hanson and Mois I. Aroyo present the server-side crystallographic programs and interactive visualizers of the *Symmetry Database* and provide examples showing how they can be used.

An appendix to the article, based on information from the *Teaching Edition* of *International Tables for Crystallography* and *International Tables for Crystallography* Volume A, provides some basic definitions and explanations of the notation used in the description of symmetry operations, coordinate transformations, and subgroups and supergroups of space groups.

We strongly urge you to read this comprehensive guide to the many different features and uses of this unique resource.

IUCR JOURNALS NEWS

Acta Cryst. A clocks up 1.25 millionth structure for the CSD



In 2019, the Cambridge Structural Database (CSD) reached 1 million structures, leading the way in structural data to inform drug discovery and materials development. Since then, the wealth of information available through the CSD has continued to grow, and in August 2023 the Cambridge Crystallographic Data Centre (CCDC) announced that the CSD had passed the milestone of 1.25 million expert-curated experimental crystal structures. We are delighted to announce that this achievement was reached with the electron diffraction structure of ibuprofen published in *Acta Crystallographica Section A: Foundations and Advances* by Malak Khouchen, Paul Klar, Hrushikesh Chintakindi, Ashwin Suresh and Lukáš Palatinus (CSD Entry: JEKNOC16). This work examines various models for the correction of estimated errors of reflection intensities in electron diffraction data, proving how one of those could notably enhance the accuracy of atomic positions and covalent bond lengths, and improve *R* factors.

In response to achieving the 1.25 millionth structure, Dr Palatinus commented,

“It is an unexpected privilege and pleasure to have helped to achieve such an important milestone for the CSD and for the whole crystallographic community.

I always illustrate the importance of crystallography to my students by reminding them that the number of published structures grows with the pace of about one structure every 10 minutes, day and night, 24/7. 1.25 million published structures is an amazing number, and I want to congratulate the whole team behind the CSD as well as to all fellow crystallographers who made this possible.

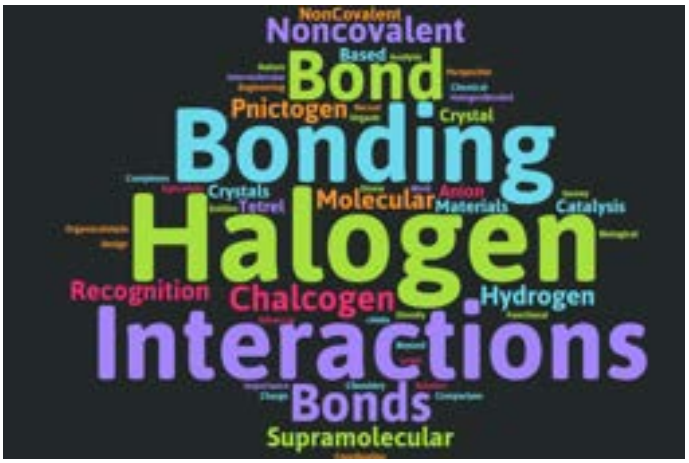
I think it is also symptomatic that the 1.25 millionth CSD structure is a structure determined by 3D electron diffraction. I believe that the number of structures determined by 3D ED in the CSD will quickly grow in the near future.”

The number of structures in the CSD measured using electron diffraction techniques is increasing rapidly. Today the CSD contains over 300 electron diffraction structures.

This article has been adapted from a CCDC blog by Giada Truccolo with permission.

IUCR JOURNALS NEWS

Exploring tetrel bonding: a special issue of Acta Cryst. C



A snapshot of current progress in the field of halogen bonds, chalcogen bonds, pnictogen bonds, tetrel bonds and other σ-hole interactions appears on the cover of the special issue. Illustration courtesy of Brammer *et al.*

Halogen bonding and related intermolecular (and sometimes intramolecular) interactions in which *p*-block elements in groups other than Group 17 serve in a Lewis acidic role have been and continue to be extensively investigated. Their applicability in supramolecular assembly is similarly well studied, with numerous reports of applications in crystal engineering, molecular recognition, catalysis, polymers and soft matter, materials chemistry, structural biology and medicinal chemistry.

This virtual special issue of *Acta Crystallographica Section C: Structural Chemistry*, titled "Halogen, chalcogen, pnictogen and tetrel bonds: structural chemistry and beyond", brings together 12 articles that cover a variety of aspects associated with halogen, chalcogen, pnictogen and tetrel bonds. The issue is introduced by a review by the Guest Editors, Lee Brammer, Anssi Peuronen and Thomas M. Roseveare. In "Halogen bonds, chalcogen bonds, pnictogen bonds, tetrel bonds and other σ-hole interactions: a snapshot of current progress", they present a compilation of review articles on σ-hole interactions published since 2013 alongside an overview of the 11 articles in the special issue on this topic.

There are articles that focus on structure, bonding and bond strength, articles that investigate co-operation or competition between different classes of interactions and articles that explore the relationship between these interactions and chemical or physical properties of the compounds and materials involved. Although all articles involve characterization by single-crystal X-ray diffraction, a number have a prominent focus on other experimental techniques or are combined with interpretation from theoretical calculations. Halogen bonding and chalcogen bonding dominate these articles, consistent with the wider literature.

EDITORIAL

A triumvirate of Section Editors moving Structural Biology Communications ahead



Figure 1. The three Section Editors of *Structural Biology Communications – Acta Cryst. F*, Cristy Nonato, Jon Agirre and Mark van Raaij.

Mark van Raaij

The IUCr and I would like to welcome Cristy Nonato and Jon Agirre as Section Editors of *Structural Biology Communications – Acta Crystallographica F*. With these appointments, we believe we have assembled a team of editors with knowledge in a wide range of structural biology disciplines and a reasonable geographical diversity (Fig. 1).

Maria Cristina Nonato (Cristy) is Full Professor at the School of Pharmaceutical Sciences of Ribeirão Preto at the University of São Paulo and coordinator of the Protein Crystallography Laboratory of Ribeirão Preto. She is President of the FCFRP Research Commission, President of the Brazilian Association of Crystallography, and Co-founder and Coordinator of the division of Structural Biology and Screening of Bioactive Compounds at the Centre for the Research and Advancement in Fragments and Molecular Targets. She is also a member of the IUCr Executive Committee.

Cristy completed her undergraduate studies in Physics and earned postgraduate degrees at the master's and doctorate levels in Applied Physics from the Institute of Physics at the University of São Paulo in São Carlos. She has 25 years of experience in structural biology, working mainly on crystallographic structure determination of proteins, enzyme kinetics, biophysical and biochemical characterization of proteins, and searching for ligands by *in vitro* and *in silico* methods as prototypes for the design of pharmaceutical drugs. She has a special interest in crystallographic fragment screening, an area of increasing importance and biomedical relevance (Martin & Noble, 2022). Cristy has co-authored more than seventy research papers, of which nine were published in IUCr journals (four in *Acta Cryst. D* and five in *Acta Cryst. F*).

Jon Agirre is a Royal Society University Research Fellow (Assistant Professor) at the Department of Chemistry at the University of York, UK. His liaisons with *Acta Cryst. F* started in 2018, guest editing a special issue on Glycoproteins and Protein–Carbohydrate Complexes, and he has been a Co-editor of the journal since 2019. He also helped edit a special issue of *Acta Cryst. D* on Model Building, Validation and Representation in MX and cryoEM. He is co-chair of CCP4 Working Group 2, a member of the CCP4 Executive Committee and the Instruct-ERIC representative on the 3D-Bioinfo (Elixir) steering committee. Jon is committed to addressing the obvious gender, racial and ethnic representation imbalances in

computational structural biology.

Career wise, Jon studied Computer Engineering at the University of the Basque Country in Donostia and completed his PhD in Biochemistry at the Unidad de Biofisica of the Spanish Research Council (CSIC) in Bilbao. He is an expert in structural bio-informatics, crystallography of glycoproteins and all that jazz (he is an aficionado of that kind of music). He is probably most well known for the program *Privateer* (Agirre *et al.*, 2015) which efficiently builds, validates and corrects carbohydrate structures. Jon has co-authored 47 research papers, of which twelve were published in IUCr journals (eleven in *Acta Cryst. D* and one in *Acta Cryst. F*), including the latest *CCP*4 general citation article (Agirre *et al.*, 2023).

Janet Newman has recently stepped down as Section Editor. We thank her for her enthusiasm and significant contributions during these last five years and hope to continue to develop her ideas for the journal. One of these ideas was to involve young scientists more, including undergraduate students – another was a more rigorous and precise description of crystallization conditions and crystallization experiments. Macromolecular crystallization is a trial without knowing the exact details of previous successful experiments carried out with similar samples. This idea can of course be extended to how samples for NMR spectroscopy and cryo-electron microscopy have been prepared.

Together, we hope to grow *Structural Biology Communications – Acta Cryst. F* as a premier journal for short but high-quality structural biology articles, covering macromolecular crystallography, cryo-electron microscopy, NMR spectroscopy and other techniques to interrogate biomolecular structure and function. Watch this space during the next few months to find out about the new ideas we have for developing the journal! And do share with us your opinions and interesting new manuscripts – Research Communications, Methods Communications and short Topical Reviews are all welcome.

References

Agirre, J., Atanasova, M., Bagdonas, H., Ballard, C. B., Baslé, A., Beilsten-Edmands, J., Borges, R. J., Brown, D. G., Burgos-Mármol, J. J., Berrisford, J. M., Bond, P. S., Caballero, I., Catapano, L., Chojnowski, G., Cook, A. G., Cowtan, K. D., Croll, T. I., Debreczeni, J. É., Devenish, N. E., Dodson, E. J., Drevon, T. R., Emsley, P., Evans, G., Evans, P. R., Fando, M., Foadi, J., Fuentes-Montero, L., Garman, E. F., Gerstel, M., Gildea, R. J., Hatti, K., Hekkelman, M. L., Heuser, P., Hoh, S. W., Hough, M. A., Jenkins, H. T., Jiménez, E., Joosten, R. P., Keegan, R. M., Keep, N., Krissinel, E. B., Kolenko, P., Kovalevskiy, O., Lamzin, V. S., Lawson, D. M., Lebedev, A. A., Leslie, A. G. W., Lohkamp, B., Long, F., Malý, M., McCoy, A. J., McNicholas, S. J., Medina, A., Millán, C., Murray, J. W., Murshudov, G. N., Nicholls, R. A., Noble, M. E. M., Oeffner, R., Pannu, N. S., Parkhurst, J. M., Pearce, N., Pereira, J., Perrakis, A., Powell, H. R., Read, R. J., Rigden, D. J., Rochira, W., Sammito, M., Sánchez Rodríguez, F., Sheldrick, G. M., Shelley, K. L., Simkovic, F., Simpkin, A. J., Skubak, P., Sobolev, E., Steiner, R. A., Stevenson, K., Tews, I., Thomas, J. M. H., Thorn, A., Valls, J. T., Uski, V., Usón, I., Vagin, A., Velankar, S., Vollmar, M., Walden, H., Waterman, D., Wilson, K. S., Winn, M. D., Winter, G., Wojdyr, M. & Yamashita, K. (2023). *Acta Cryst.* D**79**, 449–461.

Agirre, J., Iglesias-Fernández, J., Rovira, C., Davies, G. J., Wilson, K. S. & Cowtan, K. D. (2015). *Nat. Struct. Mol. Biol.* **22**, 833–834.

Martin, M. P. & Noble, M. E. M. (2022). *Acta Cryst.* D**78**, 1294–1302.

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EDITORIAL

Shaping the future of Acta Crystallographica F: unveiling our vision



Maria Cristina Nonato

As one of the Main Editors of *Acta Crystallographica F – Structural Biology Communications*, I am delighted to share our exciting plans and vision for the future of our journal. *Acta Cryst. F* has long been a cornerstone in the structural biology community, and our commitment to excellence remains unwavering.

Embracing innovation. In the ever-evolving landscape of scientific publishing, *Acta Cryst. F* is poised to embrace innovation. We are dedicated to incorporating cutting-edge technologies, data visualization tools and interactive features, such as interviews with authors, to enhance the reader's experience. Our goal is to create a dynamic platform that not only disseminates research but also fosters engagement and collaboration within the structural biology community.

Diverse and inclusive content. Recognizing the importance of diversity in scientific research, *Acta Cryst. F* aims to amplify underrepresented voices in structural biology. We will actively seek contributions that reflect a broad spectrum of perspectives, methodologies and applications. By doing so, we hope to enrich the journal's content and provide a more comprehensive view of the field.

Special issues and focus sections. To address emerging trends and interdisciplinary collaborations, *Acta Cryst. F* will introduce special issues and focus sections. These thematic collections will delve into specific areas of structural biology, such as fragment screening by X-ray crystallography, artificial intelligence methods for structure prediction and more, showcasing in-depth analyses, reviews and breakthroughs. We encourage researchers to propose topics for these special issues to ensure a wide-ranging coverage of the field.

Enhanced review and publication processes. Recognizing the value of your time and contributions, we are working to streamline our review and publication processes. Our aim is to provide faster and more transparent feedback to authors while maintaining the high standards of quality that *Acta Cryst. F* is known for.

Engaging with early career researchers. Acta Cryst. F is committed to nurturing the next generation of structural biologists. We will introduce author workshops and dedicated sections for early career researchers. Fostering a supportive environment for budding scientists is crucial for the sustained growth of our field.

Community feedback and involvement. Your input is invaluable. *Acta Cryst. F* will actively seek feedback from the structural biology community through surveys and social media interactions. We believe that

involving our readership in shaping the journal’s direction is fundamental to its success. Moreover, we plan to leverage social media platforms for enhanced visibility and engagement, ensuring that our valuable content reaches a broader audience.

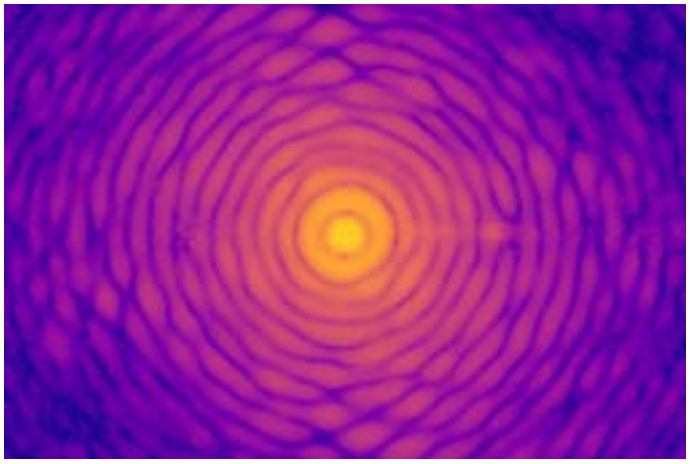
In conclusion, the future of *Acta Cryst. F* is bright, dynamic and collaborative. We invite you to embark on this journey with us as we work towards advancing structural biology and pushing the boundaries of scientific publishing.

Thank you for your continued support.

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EDITORIAL

Introduction to the special issue related to the 18th International Small Angle Scattering Conference (SAS2022)



The cover of the special issue shows a coherent small-angle X-ray scattering pattern of a zeolite crystal collected at the Cateretê beamline at Sirius, Brazil.

Florian Meneau, Jill Trewhella, Jan Ilavsky

The 18th triennial meeting of the Small Angle Scattering conference (SAS2022) was held at the Brazilian Synchrotron Light Laboratory (LNLS), part of the Brazilian Center for Research in Energy and Materials (CNPEM). In-person participants were hosted at the Royal Palm Hall Convention Center in Campinas-SP, from 11 to 16 September 2022. COVID restrictions that led to the delay in the 26th Congress and General Assembly of the International Union of Crystallography (IUCr) from 2020 to 2021 meant that this conference also was delayed by one year, and its traditional format (in-person only) was modified to support remote attendance and presentations.

The triennial SAS meeting is a major event for the international small-angle scattering community, consistently attracting hundreds of attendees from around the world [see Trewhella (2021)]. Overall, 327 participants from around the globe participated in the SAS2022 meeting, with 177 in person and 150 remote attendees. The five-day conference included 165 oral presentations, with seven plenaries plus one plenary talk given by the recipient of the 2022 Guinier Prize, Professor Jill Trewhella (https://www.iucr.org/resources/commissions/small-angle-scattering/guinier-prize). The conference Chair was Florian Meneau from the Brazilian Synchrotron Light Laboratory (LNLS). Members of the Scientific Program Committee included Aldo Craievich, Carla Polo, Celso Santilli, Cristiano Oliveira, Izabel Riegel-Vidotti, Karim Dahmouche, Mario Murakami, Mateus Cardoso, Nadya Pesce da Silveira, Renata Kaminski, Rosiane Lopes da Cunha, Watson Loh and Yraima Cordeiro. The conference program covered the field of small-angle scattering from technique development to fundamental research in materials and biology, ranging from the design and characterization of hard and soft materials to medical- and bio-technology applications. Detailed information about SAS2022, plenary sessions, a list of abstracts, videos and other details can be found at the conference web site, https://pages.cnpem.br/sas2022/.

The location of the SAS2022 conference was selected at the SAS2015 meeting in Berlin, with a major attraction being co-location with one of the first fourth-generation synchrotrons, Sirius, which recently came online in Brazil. These fourth-generation synchrotron sources, currently coming online across the globe, offer a generational upgrade in synchrotron beam qualities, such as coherence and collimation. In addition to the improved beam qualities, these sources offer increased brightness and tunability, allowing

researchers to tailor the energy and wavelength of the synchrotron radiation to suit their specific experimental needs. The enhanced collimation of the synchrotron beams allows for better control of the beam size and divergence, resulting in higher resolution and improved signal-to-noise ratio. These features enable the development of a new generation of small-angle scattering instruments, which will offer new capabilities for scientific research and development with enhanced performance for studying the structure and dynamics of materials from the nanoscale to microscale levels.

The scientific publishing landscape has evolved considerably in recent years, with the growing opportunities – and often requirements – of open-access publications. Open access has the advantage of research results being freely available to the scientific communities and leads to higher visibility and citations of the published works. Since 2012, the organizers of SAS meetings have organized the publication of special issues in *Journal of Applied Crystallography* to highlight the work presented at the meeting. The SAS2015 special issue enjoyed generous support for open access from the IUCr, and this tradition is continuing with SAS2022.

The 19 articles composing this SAS2022 special issue (https://journals.iucr.org/special_issues/2023/sas2022/) were carefully selected and represent the wide variety of topics from the meeting. The submitted manuscripts were subjected to the same rigorous review process as regular articles submitted to *Journal of Applied Crystallography*, guaranteeing high quality. The articles have been published in recent regular issues (mostly in *Journal of Applied Crystallography* with an additional article in *Acta Crystallographica Section D*) and are now combined to constitute the SAS2022 virtual special issue which highlights some of the most exciting work presented at the meeting. We are very grateful to all the authors and reviewers for their efforts that have made this high-quality special issue possible. With the rigorous selection process applied, we trust that this special issue and the 19 selected articles will provide a valuable reference for the current state-of-the-art small-angle scattering research for many years to come.

Critical to the success of our small-angle scattering community – and of any SAS conference – are sponsors and exhibitors who contribute generously to the conference program, social events and financial success. Major supporters of any SAS conference are always local grant agencies – for SAS2022 these were the Brazilian funding agencies FAPESP (2022/054006), CAPES and CNPq. Traditional and reliable community support was provided by the IUCr via travel awards (Young and Early Career Scientists Awards) and funding of the Guinier Prize. And for industrial support, despite the significant challenges of COVID travel disruptions and the hybrid conference model, our sponsors and exhibitors came in force and wholeheartedly supported our community. Their participation and sponsorship are further evidence of the health of our small-angle scattering community. While our supporters are too many to list here, we would especially like to thank our Gold sponsors: Xenocs, AVS and Anton Paar.

No conference can succeed without the tireless work of a strong local organizing committee and support staff. The necessary late decision to have SAS2022 offer hybrid participation added considerably to the burden on the local support staff, and the flawless execution has been remarked upon by many appreciative participants. We wish to deeply thank the CNPEM communication group and the Cateretê team, in particular Dora Maria Marques, Ariane de Freitas Almeida, Priscila Cassiano Alves and Murilo Silva de Oliveira.

The next triennial SAS conferences, SAS2024 and SAS2027, will be held in Taiwan and Sweden, respectively. We wish the organizers of these meetings the very best for their respective conferences.

Acknowledgements

We thank Charles S. Bond, University of Western Australia, for editing the article that originally appeared in *Acta Crystallographica Section D*. We also thank everyone at the IUCr Editorial Office for their kind support in the preparation of this special issue. We gratefully acknowledge the generous support provided by the IUCr through travel scholarship support for the SAS2022 conference.

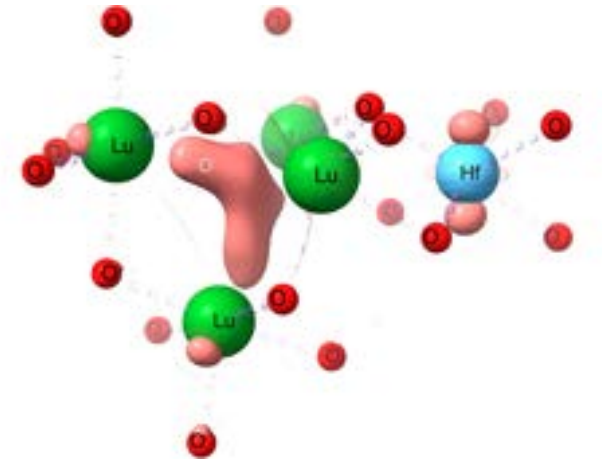
References

Trewhella, J. (2021). *J. Appl. Cryst.* **54**, 1029–1033.

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COMMENTARY

Electron traps and energy storage: modeling a bright path to the future



Renaldo T. Moura Jr

The luminescence phenomenon manifests when a substance emits light without undergoing heating. This occurrence is typically initiated through the excitation of the substance by various forms of energy. Light, serving as an excitation source, is capable of inducing luminescence, and in such cases, the exciters are referred to as phonons, giving rise to what is known as photoluminescence. It is noteworthy that alternative excitation sources exist, as discussed by Kulesza *et al.* (2016), such as electric current (resulting in electroluminescence), electron beam exposure (leading to cathodoluminescence), energy released during a chemical reaction (resulting in chemiluminescence), mechanical action (causing mechanoluminescence), ionizing radiation (yielding radioluminescence), and even changes in temperature, either through heating (thermoluminescence) or cooling (cryoluminescence), among others.

In all instances, the excitation source serves the purpose of promoting electrons that, within a brief period, undergo recombination, thereby giving rise to the luminescence phenomenon. Notably, materials exhibiting an extended duration of glow subsequent to the cessation of excitation are characterized as having persistent luminescence (Xu & Tanabe, 2019). The gradual release of excited electrons can be classified as a form of energy storage. This particular phenomenon involves the presence of energy traps, such as electron or hole traps, within a material, which are occupied during the excitation process. Understanding this phenomenon poses a challenge due to the conventional treatment of solid-state systems under the non-localized regime of conduction and valence band structures. Consequently, conceiving of a trap that completely localizes electrons becomes difficult in this context.

The challenge of localization is not novel in solid-state chemistry. In 1997, Marzari and colleagues introduced the Maximally Localized Wannier Functions (MLWF) method, presenting an alternative avenue for analyzing chemical bonding in periodic systems (Marzari & Vanderbilt, 1997; Silvestrelli *et al.*, 1998; Souza *et al.*, 2001; Marzari *et al.*, 2012). MLWFs replace the traditional non-localized Bloch wavefunctions, serving to localize the band structure into MLWF orbitals. Additionally, the Crystal Orbital Hamiltonian Population (COHP) method (Dronskowski & Bloechl, 1993) and the Crystal Orbital Overlap Population (COOP) method (Hughbanks & Hoffmann, 1983) offer an alternative means of characterizing chemical bonds in periodic systems (Ruggiero *et al.*, 2015). These two techniques share almost identical formulations and operate in a similar way to conventional Density of States (DOS) calculations. However, instead of considering contributions from all orbitals in a molecular or periodic system, they facilitate the examination of specific interaction pairs between two sets of orbitals (Ruggiero *et al.*, 2017). Both COOP and COHP schemes allow for the quantification of orbital overlap and the strength of interatomic bonds

(Rohling *et al.*, 2019). These methods provide valuable insights into the bonding characteristics of periodic systems, delivering a detailed analysis of specific orbital interactions and exemplifying effective localization tools for such systems.

The work of Andrii Shyichuk (2023) (in this issue of *Acta Crystallographica Section B*) is truly inspiring, particularly in its exploration of the localization of electron traps in doped materials. Employing a time-dependent extension of density functional theory – a widely used framework in solid-state chemistry and physics – Shyichuk significantly advances our understanding of the behavior of an oxygen vacancy in cubic lutetium oxide (c-Lu_2O_3). The study delves into the impact of dopants such as Hf or Zr on the electron density trapped within the vacancy.

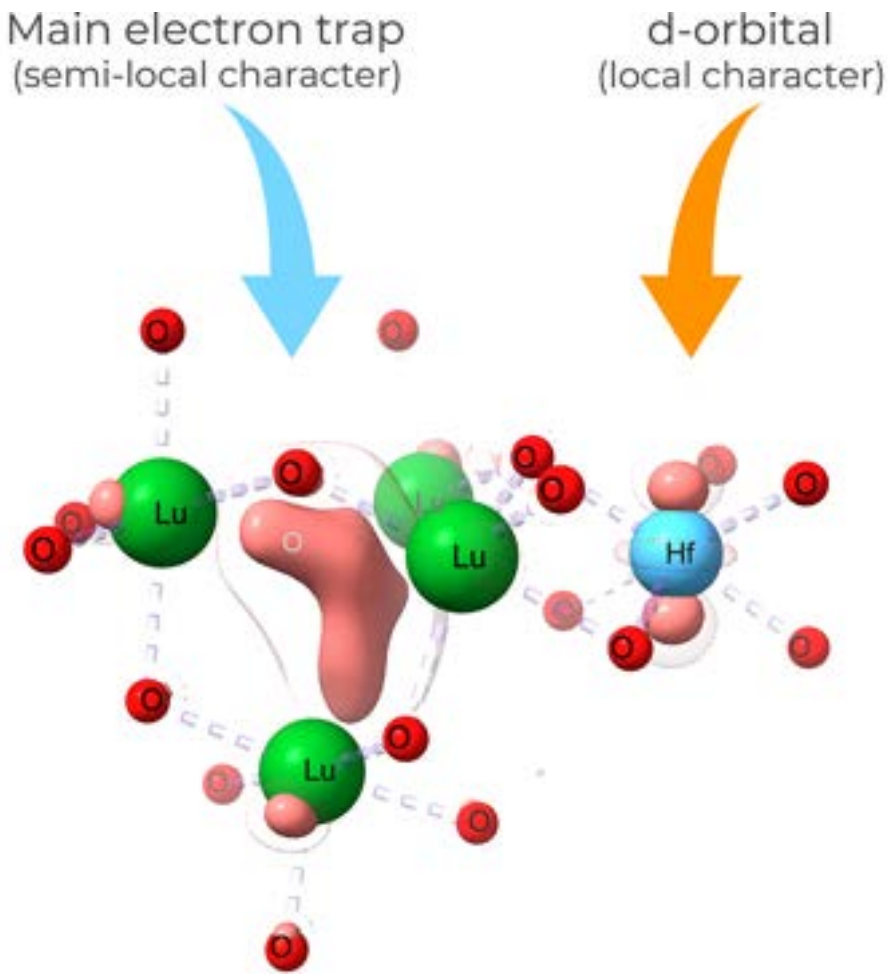


Figure 1. Trapped electron density as obtained by Shyichuk (2023) for an oxygen vacancy in Lu_2O_3:Hf. Isosurfaces have contour values of 0.004 and 0.009 e a_0^{-3}. Structure and electron density maps were created using the *ChimeraX* software (Pettersen *et al.*, 2021; Goddard *et al.*, 2018).

The results presented by Shyichuk offer intriguing and insightful findings, exemplified by the localized behavior of the trapped electron (see Fig. 1). The study demonstrates that the trapped electron density not only occupies the vacancy site with a semi-local character (as illustrated on the left-hand side of Fig. 1) but also engages *d*-type orbitals in elements such as Hf (as depicted on the right-hand side of Fig. 1). This nuanced understanding is thoroughly discussed, shedding light on the multifaceted nature of electron trapping in doped materials.

In the context of phosphors, Yen *et al.* (2007) emphasize the importance of addressing various facets such as lattice relaxation, charge-compensating defects, intrinsic defects, the nature of the bottom of the conduction band, and the dynamic properties involved in charge localization and delocalization processes, along with theoretical modeling. Moreover, Yen is acknowledged (Kulesza *et al.*, 2016) for asserting that the conceivable applications of these materials are limited solely by the innovative capacity of individuals engaged in research and development.

In this context, the work of Shyichuk (2023) is deemed a milestone. This designation is warranted as Shyichuk's research significantly contributes to the understanding of electron/hole traps in doped materials. By exploring the intricacies of electron/hole traps, Shyichuk's work extends the boundaries of knowledge, fostering an expanded imagination among readers. This contribution not only advances our comprehension of these materials but also illuminates a promising path toward the development of more energy-efficient materials.

Acknowledgements

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References

Dronskowski, R. & Bloechl, P. E. (1993). *J. Phys. Chem.* **97**, 8617–8624.

Goddard, T. D., Huang, C. C., Meng, E. C., Pettersen, E. F., Couch, G. S., Morris, J. H. & Ferrin, T. E. (2018). *Protein Sci.* **27**, 14–25.

Hughbanks, T. & Hoffmann, R. (1983). *J. Am. Chem. Soc.* **105**, 3528–3537.

Kulesza, D., Bolek, P., Bos, A. J. J. & Zych, E. (2016). *Coord. Chem. Rev.* **325**, 29–40.

Marzari, N., Mostofi, A. A., Yates, J. R., Souza, I. & Vanderbilt, D. (2012). *Rev. Mod. Phys.* **84**, 1419–1475.

Marzari, N. & Vanderbilt, D. (1997). *Phys. Rev. B*, **56**, 12847–12865.

Pettersen, E. F., Goddard, T. D., Huang, C. C., Meng, E. C., Couch, G. S., Croll, T. I., Morris, J. H. & Ferrin, T. E. (2021). *Protein Sci.* **30**, 70–82.

Rohling, R. Y., Tranca, I. C., Hensen, E. J. & Pidko, E. A. (2019). *J. Phys. Chem. C*, **123**, 2843–2854.

Ruggiero, M. T., Erba, A., Orlando, R. & Korter, T. M. (2015). *Phys. Chem. Chem. Phys.* **17**, 31023–31029.

Ruggiero, M. T., Sibik, J., Erba, A., Zeitler, J. A. & Korter, T. M. (2017). *Phys. Chem. Chem. Phys.* **19**, 28647–28652.

Shyichuk, A. (2023). *Acta Cryst.* B**79**, 437–449.

Silvestrelli, P. L., Marzari, N., Vanderbilt, D. & Parrinello, M. (1998). *Solid State Commun.* **107**, 7–11.

Souza, I., Marzari, N. & Vanderbilt, D. (2001). *Phys. Rev. B*, **65**, 035109.

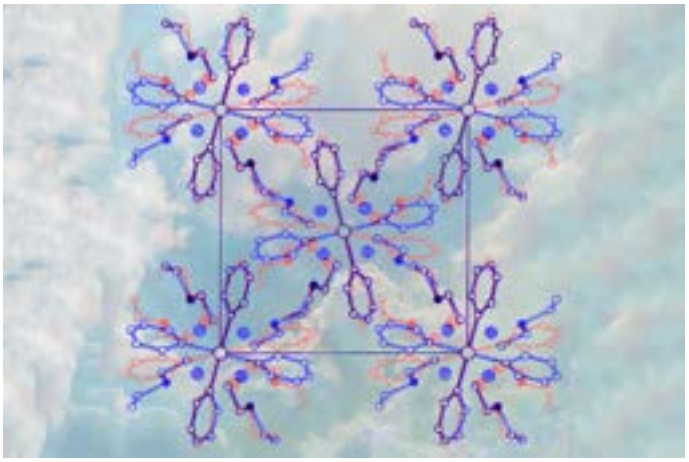
Xu, J. & Tanabe, S. (2019). *J. Lumin*. **205**, 581–620.

Yen, W. M., Shionoya, S. & Yamamoto, H. (2007). Editors. *Phosphor Handbook*, 2nd ed. Boca Raton: CRC Press.

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COMMENTARY

Mythical compounds



Phillip E. Fanwick

As crystallography became readily available, it was obvious there was a need for validation methods to ensure the quality and consistency of the reported data. While there were several publications indicating this need, the publication that really provided the impetus was entitled *Some Incorrect Space Groups* in Volume 16 of *Inorganic Chemistry* by Richard Marsh and Verner Schomaker (Marsh & Schomaker, 1979). Dick Marsh continued publishing similar lists of incorrect space groups for many years and in fact being cited in such a publication was referred to as 'being Marshed'. The only problem discussed in these publications was the choice of space group, though some required a change in the Laue class. If something so basic to crystallography as the space group was not being determined correctly, one could only imagine the extent of other problems. Collecting crystallographic data, structure solution and structure refinement required the crystallographer to make many decisions. Frequently, the researcher will be biased towards a desired result and may force the structure to be consistent with the expected model. It was obvious some program was needed to check results.

However, before validation programs could be written, a universal formatted output from crystallographic experiments was needed. The program would provide a means to report all the crystallographic data, as well as the metadata, which could help in validating the methods used and ensure all the required data were provided. This required output was the crystallographic information file (CIF) format (Hall *et al.*, 1991).

With the development of CIF, it was now possible to create software that could carry out validation of crystal structures. The most widely used such software is *checkCIF* by Ton Spek (Spek, 2020). This program was first reported in 2003 (Spek, 2003) and has found widespread use ever since. The program provided an extensive validation of submitted data and found widespread adoption. Once instituted, many complained of the problems of generating CIFs and understanding and correcting the errors *checkCIF* reported. However, both CIF and *checkCIF* have proved vital to the growth of good crystallography. Many reports of questionable or incorrect crystallography have been caught before they entered the literature and they alerted many producing and publishing crystallographic results to potential problems.

The use of crystal structure validation has led to the assumption that validation to ensure that the crystallographic results are correct means the chemical results must also be correct. An article by Kenneth Raymond and Gregory Girolami (Raymond & Girolami, 2023) proves that this assumption is incorrect. This article reviews published reports that all contain inaccurate chemical conclusions. These structures were published in science journals which are all peer reviewed. The erroneous structures were published from 1976 to 2019, so, in most cases, current software and diffractometers were used. The majority were published after 1999. Not surprisingly, many of these structures were offered as reports of

new or highly unusual compounds which later proved to be non-existent.

Raymond and Girolami note several classes of chemically incorrect structures. The first class is the obvious case of structures with incorrectly assigned atoms. The second is high-symmetry superstructures which include guest molecules. The third class is cases of an incorrectly assigned space group which also results in incorrect crystallography. The last case is that of incorrectly determined unit cells, again a crystallographic error.

Included with all the incorrect results presented by Raymond and Girolami are brief discussions of why the results are wrong and explanations or, in some cases, speculation as to how they ended up with incorrect chemistry. The most chemically incorrect structure is a report of a series of new divalent lanthanide compounds $Ni_2[LnCl_6]$ (Ln = Eu, Ce and Gd) (Baldo *et al.*, 2018). All turned out to be the complex $[Ni(NH_3)_6]^{2+}$ with a disordered anion of chloride and nitrate. By coincidence, the three elements Ln, Ni and Cl all have atomic numbers about 2.3 times greater than the actual elements of Ni, a mixture of Cl and N, and N. Since the ratio of the atomic numbers was nearly the same in both the correct and incorrect formulation, the structures refined because the scale factor was able to adjust for the incorrect number of electrons.

It is clear that just validating the crystallography is insufficient to ensure the correctness of the formula, connectivity and geometric parameters from structural determinations. Hopefully this article by Raymond and Girolami will alert and alarm chemists, crystallographers, referees and editors of the need to not always trust the crystal structure but also to ensure that the chemistry is consistent with previous chemistry. This is especially true for reports of new or totally unexpected compounds. Maybe it will encourage some in the crystallographic community (if it is not already being done) to try to apply the advances in artificial intelligence using the copious amount of data in the various crystallographic databases to create a chemistry validation program for crystal structures. David Watkin of Oxford University has frequently labeled crystallography as the 'Gold Standard' of analytical methods. More must be done to ensure in the future it will not lose its luster.

References

Baldo, B., Rubio, F., Flores, E., Vega, A., Audebrand, N., Venegas-Yazigi, D. & Paredes-García, V. (2018). *Chem. Commun.* **54**, 7531–7534.

Hall, S. R., Allen, F. H. & Brown, I. D. (1991). *Acta Cryst.* A**47**, 655–685.

Marsh, R. E. & Schomaker, V. (1979). *Inorg. Chem.* **18**, 2331–2336.

Raymond, K. N. & Girolami, G. S. (2023). *Acta Cryst.* C**79**, 445–455.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

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COMMENTARY

Predicting photoactivity in dithienylethene crystalline solids



Kristin M. Hutchins

Stimuli-responsive materials are a unique class of compounds that undergo a change in response to an applied stimulus. Common stimuli include light, temperature, force and chemical, while the response of the material to such stimuli can vary widely, including changes in shape, color and stiffness, among others (Li, Iscen *et al.*, 2020; Roy *et al.*, 2010; Yan *et al.*, 2022; Yang *et al.*, 2023). Materials that respond to stimuli have attracted attention because they can provide information about the environment around them. For example, materials that exhibit color changes can be used for *anti*-counterfeiting, changing lenses or to indicate applied force (Li, Huang *et al.*, 2020; Malic *et al.*, 2010; Qian *et al.*, 2021). At the molecular level, these changes typically arise from a change in structure, which is initiated by the stimulus.

Photoswitchable materials contain a molecule that is capable of changing its structure in response to the application of light as a stimulus. For solid or crystalline phase materials, there are typically requirements that need to be met for the molecule to be photoactive and undergo a structural change because motion in solids is more restricted. Dithienylethenes are one class of photoswitchable materials that can be converted between an open and closed form, depending on exposure to certain wavelengths of light [Fig. 1(*a*)]. Dithienylethenes are promising candidates for incorporation into organic photoswitches because they react in the solid state, both forms are thermally stable, and they are resistant to fatigue (Herder *et al.*, 2015; Kitagawa *et al.*, 2013; Kobatake *et al.*, 2000; Shibata *et al.*, 2002). For a dithienylethene to be considered potentially photoactive in the solid state, the molecule should adopt an antiparallel geometry and the two active carbon atoms should have an interatomic distance of less than 4.2 Å (Kobatake *et al.*, 2002). However, the conformational flexibility of dithienylethenes (via free rotation of thiophene rings) creates challenges in designing and achieving conformations that are photoactive in the solid state. In this issue of **IUCrJ**, Benedict and coworkers take on this challenge by preparing several solid-state forms of a dithienylethene derivative and developing a facile and robust analysis method that can be used to predict photoreactivity in the system (Mitchell *et al.*, 2023). By pairing experimental crystal structure data with calculations, the described method provides an easy way to relate structure to property. Importantly, the method could be applied more broadly to other dithienylethene systems to predict solid-state photoactivity.

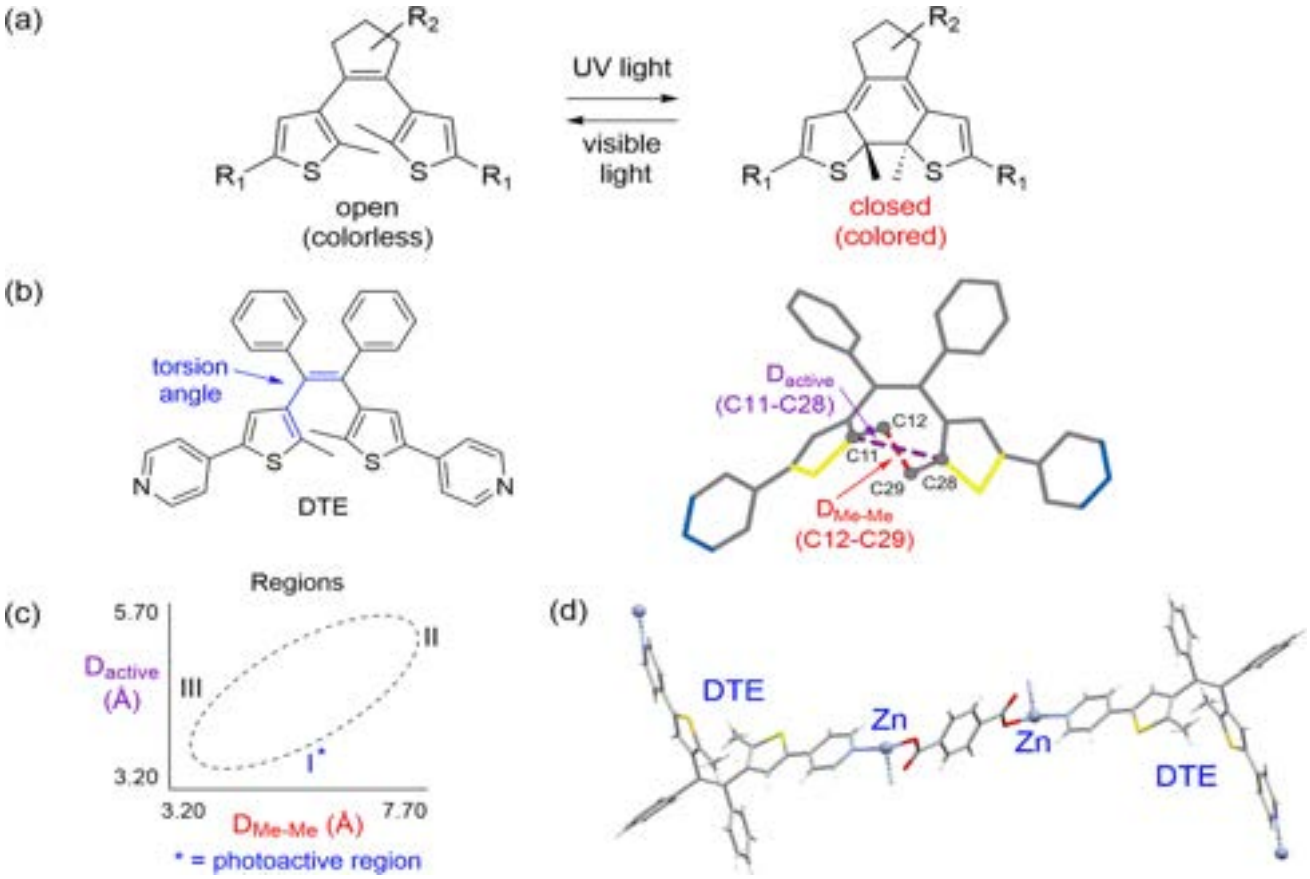


Figure 1. (*a*) General dithienylethene structure in open and closed form. (*b*) Pyridyl-functionalized dithienylethene derivative (DTE) highlighting atoms used in torsion angle measurements (blue), the distance between active carbons (D_{active}) and the distance between methyl groups ($D_{Me–Me}$) (Mitchell *et al.*, 2023). (*c*) Plot of D_{active} versus $D_{Me–Me}$ showing locations of the three distinct and populated regions. (*d*) One of the two photoactive compounds obtained with DTE.

Crystal engineering, the rational design of functional molecular solids (Desiraju, 1995; Etter, 1990; Metrangolo *et al.*, 2005; Moulton & Zaworotko, 2001; Schmidt, 1971), offers a strategy for obtaining solid-state structures that are expected to be photoactive. However, if there are few structures known, or if suitable design strategies have not been developed for a given class of molecules, 'engineering' the solid to exhibit a desired structure, and thus function, becomes more challenging. Therefore, the development of structural landscapes for such classes of molecules is useful (Desiraju, 2017, 2021). By determining several structures and taking each structure as a data point on the landscape, structure–property relationships can be developed.

In the article by Benedict and coworkers, the crystal structure landscape of the molecule (*Z*)-1,2-bis-[2-methyl-5-(pyridin-4-yl)thiophen-3-yl]-1,2-diphenylethene, abbreviated 'DTE', is investigated [Fig. 1(*b*), left]. By incorporating DTE into a variety of solids, and thus obtaining several data points, the authors aim to gain a broad understanding of behavior and develop the structural landscape. Specifically, the authors investigate an array of compound types including the parent compound, hydrogen-bonded cocrystals and coordination compounds. The parent compound, DTE, is polymorphic and two structures were obtained. Through cocrystallization with multitopic carboxylic acids, four hydrogen-bonded cocrystals were prepared. Six coordination polymers were synthesized with DTE as a ligand. Finally, seven solids were obtained from metal–organic framework syntheses using zinc, DTE and multitopic carboxylic acids. In total, 19 structures were used to form the basis of the structural landscape for this pyridyl-functionalized dithienylethene derivative.

Using established requirements for photoactivity in dithienylethene compounds (*i.e.* antiparallel geometry and an interatomic distance less than 4.2 Å), the authors visually examined each DTE molecule within each solid-state structure. Within the 19 solids, 17 contained photoinactive DTE molecules and two contained photoactive DTE molecules. Considering the broad class of compounds prepared in the study,

the work shows that obtaining photoactive conformations in the solid state is not trivial.

The authors conducted relaxed potential energy surface scans using a geometry-optimized DTE molecule, and the torsion angle [Fig. 1(*b*), blue atoms] was rotated through ±1° increments to create a 360° analysis of the molecule with corresponding energies for each position. These calculations afforded four energetic minima overall, which correspond to four unique conformations, two antiparallel and two parallel. Since an antiparallel arrangement is required for photoactivity, the authors looked at the distance between the active carbons in the two minimum energy antiparallel conformations. One conformation had an interatomic distance of 3.45 Å, while the second was 5.19 Å; thus, only the former conformation would be expected to be photoactive. The authors mention that visual inspection of conformers can be time-consuming and somewhat subjective; thus, they sought to develop a simple method to determine conformer type and photoactivity potential unambiguously.

The first parameter they define is D_{active}, which is simply the measured distance between the active carbons, and the distance should be less than 4.2 Å to be photoactive. The second parameter they define is $D_{\text{Me–Me}}$, which is the distance between the two methyl groups on the thiophene rings [Fig. 1(*b*), right]. $D_{\text{Me–Me}}$ will give values that are invariable with respect to structure inversion, *i.e.* enantiomers would afford identical values. Plotting the values of D_{active} versus $D_{\text{Me–Me}}$ using the calculated structures affords a broken ellipse shape, with three distinct areas that are populated [Fig. 1(*c*)]. The regions include: (I) antiparallel conformations with $D_{\text{active}} < 4.2$ Å, (II) antiparallel conformations with $D_{\text{active}} > 4.2$ Å and (III) parallel conformations. Moreover, when the experimentally obtained values from the 19 unique X-ray crystal structures are added to the plot, they also fall into the same three regions. The two synthesized DTE solids that were experimentally photoactive fall into region I, which is indeed the expected photoactive region [Fig. 1(*d*)].

This work demonstrates the power of experiment and theory conducted in tandem for predicting properties in crystalline materials. The D_{active}–$D_{\text{Me–Me}}$ analysis provides a straightforward way to predict photoactivity using only two distance measurements. Rapid and effective tools, such as the analysis method described, are valuable to the crystal engineering community. First, such tools are useful to understand why a given structure affords a property. Second, and where the tool shows effectiveness, is when it can be used with crystal engineering strategies to design materials that exhibit desired solid-state conformations and corresponding properties. Further application of this tool to DTE and other dithienylethene derivatives will aid in achieving photoactive conformations (and photoswitching) in the solid state.

References

Desiraju, G. R. (2017). *Acta Cryst.* B**73**, 775–778.

Desiraju, G. R. (2021). *IUCrJ*, **8**, 148–149.

Desiraju, G. R. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2311–2327.

Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.

Herder, M., Schmidt, B. M., Grubert, L., Pätzel, M., Schwarz, J. & Hecht, S. (2015). *J. Am. Chem. Soc.* **137**, 2738–2747.

Kitagawa, D., Nishi, H. & Kobatake, S. (2013). *Angew. Chem. Int. Ed.* **52**, 9320–9322.

Kobatake, S., Shibata, K., Uchida, K. & Irie, M. (2000). *J. Am. Chem. Soc.* **122**, 12135–12141.

Kobatake, S., Uchida, K., Tsuchida, E. & Irie, M. (2002). *Chem. Commun.* pp. 2804–2805.

Li, C., Iscen, A., Palmer, L. C., Schatz, G. C. & Stupp, S. I. (2020). *J. Am. Chem. Soc.* **142**, 8447–8453.

Li, W., Huang, Q., Mao, Z., Zhao, J., Wu, H., Chen, J., Yang, Z., Li, Y., Yang, Z., Zhang, Y., Aldred, M. P. & Chi, Z. (2020). *Angew. Chem. Int. Ed.* **59**, 3739–3745.

Malic, N., Campbell, J. A., Ali, A. S., York, M., D'Souza, A. & Evans, R. A. (2010). *Macromolecules*, **43**, 8488–8501.

Metrangolo, P., Neukirch, H., Pilati, T. & Resnati, G. (2005). *Acc. Chem. Res.* **38**, 386–395.

Mitchell, T. B., Zhang, X., Jerozal, R. T., Chen, Y.-S., Wang, S. & Benedict, J. B. (2023). *IUCrJ*, **10**, 694–699.

Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.

Qian, H., Purwanto, N. S., Ivanoff, D. G., Halmes, A. J., Sottos, N. R. & Moore, J. S. (2021). *Chem*, **7**, 1080–1091.

Roy, D., Cambre, J. N. & Sumerlin, B. S. (2010). *Prog. Polym. Sci.* **35**, 278–301.

Schmidt, G. M. J. (1971). *Pure Appl. Chem.* **27**, 647–678.

Shibata, K., Muto, K., Kobatake, S. & Irie, M. (2002). *J. Phys. Chem. A*, **106**, 209–214.

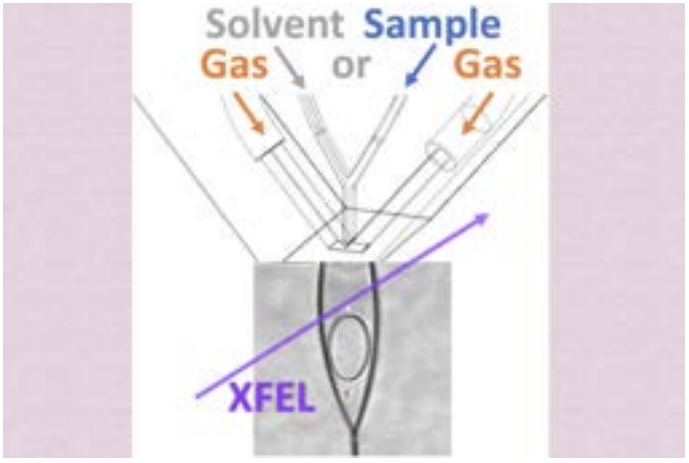
Yan, D., Wang, Z. & Zhang, Z. (2022). *Acc. Chem. Res.* **55**, 1047–1058.

Yang, X., Lan, L., Pan, X., Di, Q., Liu, X., Li, L., Naumov, P. & Zhang, H. (2023). *Nat. Commun.* **14**, 2287.

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COMMENTARY

Thinner than a knife's edge: 3D-printed liquid sheet jet technology for solution phase XFEL experiments



Martin Trebbin

The unique characteristics of X-ray free-electron lasers (XFELs) have opened new experimental frontiers for the life and materials sciences. This has enabled the development of novel methods, such as serial femtosecond crystallography (SFX), fluctuation X-ray scattering (FXS) and several X-ray spectroscopies, which have transformed atomic resolution molecular imaging and ultrafast materials characterization (Chapman *et al.*, 2011; Kraus *et al.*, 2018; Bergmann *et al.*, 2021; Konold *et al.*, 2023). The XFELs' ultrashort X-ray pulses with exceptional peak brilliance and spatial coherence allow us to record molecular movies of chemical and biological processes with unprecedented spatial and temporal resolution. These exciting possibilities come at a hefty price, however: the sample typically gets *blown up* or heavily modified by the intense X-ray dose (Neutze *et al.*, 2000; Stan *et al.*, 2016). Although the diffraction-before-destruction principle still allows damage-free data collection at room temperature at XFELs (Chapman *et al.*, 2011), the sample must be swiftly and efficiently replaced before the next X-ray pulse arrives. While the limited availability of most biological samples already complicates the technical realization of this requirement, the introduction of MHz-rate XFELs further exacerbates the challenge (Wiedorn *et al.*, 2018*b*; Grünbein *et al.*, 2018; Sobolev *et al.*, 2020). Furthermore, the produced data must be of the highest possible quality and collected with maximum efficiency regarding sample and beamtime use (Konold *et al.*, 2023). Thus, the effective and efficient investigation of liquid phase sample specimens with high-precision X-ray techniques still represents a unique challenge for XFELs (Konold *et al.*, 2023).

At present, the gas-dynamic virtual nozzle (GDVN) is predominantly utilized for liquid sample injection in XFELs (DePonte *et al.*, 2008; Vakili *et al.*, 2020; Vakili *et al.*, 2022; Knoška *et al.*, 2020; Nazari *et al.*, 2020; Nelson *et al.*, 2016; Trebbin *et al.*, 2014). In brief, a microscopic liquid stream is sheathed and accelerated by a stream of pressurized gas, forming a few-micron-wide liquid jet that is ejected in the vacuum (Gañán-Calvo, 1998; DePonte *et al.*, 2008). The resulting cylindrical liquid jet must reach velocities on the order of tens of m s^{-1} to outpace radiation-induced sample explosions from consecutively incoming X-ray pulses (Stan *et al.*, 2016; Wiedorn *et al.*, 2018*a*; Wiedorn *et al.*, 2018*b*). Today, these GDVNs are typically produced via high-resolution 3D printing, such as two-photon polymerization (Oberthuer *et al.*, 2017; Knoška *et al.*, 2020), yielding reproducible channel geometries that allow the minimization of sample flow rates, scattering background from the solvent, and reduce extreme sample consumption. However, this GDVN approach comes with longstanding issues severely impacting the success rate of XFEL experiments, such as vacuum compatibility issues, susceptibility to

clogging and large background fluctuations (Konold *et al.*, 2023). The latter challenge primarily stems from the X-ray beam pointing fluctuations hitting the cylindrical liquid jet: with typical jet diameters of *ca* 3 µm, slight deviations from the jet center result in significant changes of the X-ray interaction volume (Eggers & Villermaux, 2008).

An emerging method to overcome many of the above challenges is the use of liquid sheets that provide a consistent thickness over large areas (Ha *et al.*, 2018; Koralek *et al.*, 2018; Hoffman *et al.*, 2022*a*; Hoffman *et al.*, 2022*b*). Originally, free-flowing liquid sheets were generated using two impinging laminar jets resulting in smooth flows and stable jetting over long periods (Taylor, 1960; Bush & Hasha, 1999). More recently, glass-based microfluidic devices made via lithography were demonstrated utilizing gas acceleration to generate dramatically thinner sheets (Koralek *et al.*, 2018; Hoffman *et al.*, 2022*a*; Hoffman *et al.*, 2022*b*). However, the use of sheet jets at XFELs has been far less prevalent due to high liquid and gas loads that complicate vacuum operation (Konold *et al.*, 2023).

In the current issue of **IUCrJ**, Konold *et al.* present a refreshing and exciting approach addressing these above challenges: a 3D-printed gas-accelerating nozzle design for the generation of thin liquid sheets providing reproducible device fabrication, excellent stability, reduced liquid flow rates, low background and compatibility with high-repetition rate XFELs (Konold *et al.*, 2023). The device performance has been thoroughly investigated at the European XFEL's SPB/SFX instrument using nanofocused X-ray scattering and highspeed video microscopy, yielding promising results for the interrogation of liquid samples at XFELs. Two of the most interesting results of this study are the large and even hit area and the achieved sheet thicknesses, as shown in Fig. 1. However, we will also shed light on some operational nuances that still have to be overcome.

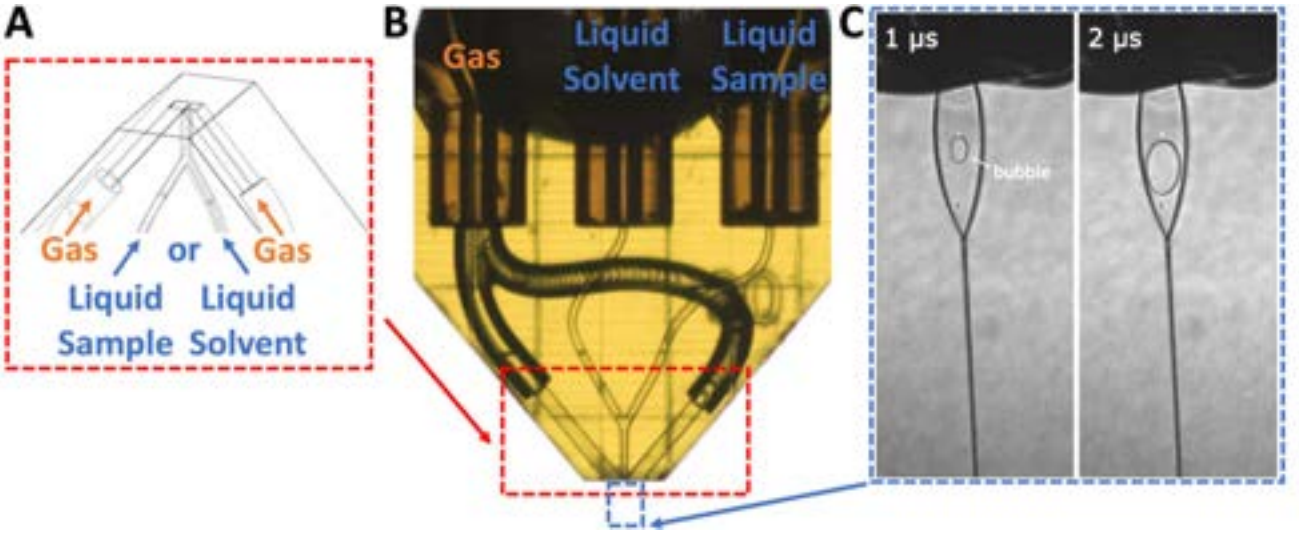


Figure 1. Konold *et al.* present a 3D-printed nozzle for the generation of sheet jets. (*A*) CAD-design of the gas-accelerated nozzle design. (*B*) A microscopic image of the 3D-printed nozzle (*ca* 1.5 mm long). (*C*) Stroboscopic images of sheet jet explosion and void formation from two consecutive XFEL pulses (141 kHz). Image adapted from Konold *et al.* (2023).

First, the flatness and large area of the generated sheet vastly reduces sensitivity to X-ray beam pointing fluctuations improving scaling characteristics. The liquid sheet also overcomes longstanding difficulties of cylindrical jets, such as the distortion of pump laser focus properties or the calculation of take-off angles for X-ray photoelectron spectroscopy (Konold *et al.*, 2023).

Second, the liquid sheet jets can be made very thin, ranging from a few hundred nanometres down to 60 nm. Compared with traditional GDVN jets, the *ca* 30-fold reduction in X-ray path length and 4-fold reduction in background offers intriguing experimental possibilities (Konold *et al.*, 2023). Specifically, the background levels for X-ray scattering and spectroscopic investigations can be dramatically reduced, approaching the single-molecule scale. The minimal, wedge-like thickness variation can be used as a feature for swiftly adjusting the sample thickness on the fly by simply translating the nozzle. One must also not forget that the reduction in interaction volumes also reduces the impact from radiation-induced explosions, resulting in perturbation-free solution scattering data collection up to 564 kHz.

While the liquid flow rate is lower than previous sheet jet devices, it remains a challenge for scarce samples, such as proteins, because the liquid flow rate is still 3- to 5-fold higher than the GDVN it was compared with (Konold *et al.*, 2023). Consequently, the vacuum compatibility of these devices remains a challenge, typically requiring differential pumping, cryo-trapping and/or heated sample catchers, which are not present at every beamline, thus limiting applicability (Konold *et al.*, 2023). However, since most of the liquid volume is found in the much thicker rims, the authors make a few suggestions on how to potentially overcome these challenges, such as reducing channel dimensions or using carrier liquids, but those solutions will require further development (Hoffman *et al.*, 2022*a*; Oberthuer *et al.*, 2017). Another aspect to consider is the parabolic velocity profile across the sheet jet resulting from the gas focusing, which might make time-resolved experiments triggered by rapid mixing challenging to evaluate (Choo & Kang, 2002).

Although the study and evaluation were carried out thoroughly and in detail, showcasing the exciting applications for sheet jets, it is noteworthy that the experiments have been carried out only with 2-propanol. Thus, it remains to be seen how these devices will perform under realistic conditions, *i.e.* with aqueous samples and buffers, which are more prone to icing and clogging, especially under vacuum conditions.

While there is still some room for improvement, the liquid sheet technology remains an exciting addition to the liquid phase sample delivery toolset at XFELs because the tremendous experimental opportunities far outweigh the remaining few challenges. The stable, low background and large flat area of liquid sheets down to tens of nanometres of thickness not only offer great opportunities for various (soft) X-ray spectroscopies (Ekimova *et al.*, 2015; Smith *et al.*, 2020; Fondell *et al.*, 2017), high-harmonic generation (Luu *et al.*, 2018) and high-intensity laser plasma investigations (George *et al.*, 2019) but also lead the way towards electron diffraction (Nunes *et al.*, 2020; Yang *et al.*, 2021) and small-/wide-angle X-ray solution scattering experiments (Blanchet *et al.*, 2023). The nanometre-thin liquid sheets with low, stable background are especially attractive for experiments which benefit from small interaction volumes, such as fluctuation X-ray scattering (Kurta *et al.*, 2017; Pande *et al.*, 2018; Konold *et al.*, 2023). With thicknesses approaching those of vitreous ice in cryo-electron microscopy, this study points towards the thrilling possibility of carrying out ultrafast single-particle solution scattering (Adrian *et al.*, 1984; Kontziampasis *et al.*, 2019; Klebl *et al.*, 2020*a*; Klebl *et al.*, 2020*b*).

References

Adrian, M., Dubochet, J., Lepault, J. & McDowall, A. W. (1984). *Nature*, **308**, 32–36.

Bergmann, U., Kern, J., Schoenlein, R. W., Wernet, P., Yachandra, V. K. & Yano, J. (2021). *Nat. Rev. Phys.* **3**, 264–282.

Blanchet, C. E., Round, A., Mertens, H. D. T., Ayyer, K., Graewert, M., Awel, S., Franke, D., Dörner, K., Bajt, S., Bean, R., Custódio, T. F., de Wijn, R., Juncheng, E., Henkel, A., Gruzinov, A., Jeffries, C. M., Kim, Y., Kirkwood, H., Kloos, M., Knoška, J., Koliyadu, J., Letrun, R., Löw, C., Makroczyova, J., Mall, A., Meijers, R., Pena Murillo, G. E., Oberthür, D., Round, E., Seuring, C., Sikorski, M., Vagovic, P., Valerio, J., Wollweber, T., Zhuang, Y., Schulz, J., Haas, H., Chapman, H. N., Mancuso, A. P. & Svergun, D. (2023). *Commun. Biol.* **6**, 1057.

Bush, J. W. M. & Hasha, A. E. (1999). *J. Fluid Mech.* **511**, 285–310.

Chapman, H. N., Fromme, P., Barty, A., White, T. A., Kirian, R. A., Aquila, A., Hunter, M. S., Schulz, J., DePonte, D. P., Weierstall, U., Doak, R. B., Maia, F. R. N. C., Martin, A. V., Schlichting, I., Lomb, L., Coppola, N., Shoeman, R. L., Epp, S. W., Hartmann, R., Rolles, D., Rudenko, A., Foucar, L., Kimmel, N., Weidenspointner, G., Holl, P., Liang, M., Barthelmess, M., Caleman, C., Boutet, S., Bogan, M. J., Krzywinski, J., Bostedt, C., Bajt, S., Gumprecht, L., Rudek, B., Erk, B., Schmidt, C., Hömke, A., Reich, C., Pietschner, D., Strüder, L., Hauser, G., Gorke, H., Ullrich, J., Herrmann, S., Schaller, G., Schopper, F.,

Soltau, H., Kühnel, K.-U., Messerschmidt, M., Bozek, J. D., Hau-Riege, S. P., Frank, M., Hampton, C. Y., Sierra, R. G., Starodub, D., Williams, G. J., Hajdu, J., Timneanu, N., Seibert, M. M., Andreasson, J., Rocker, A., Jönsson, O., Svenda, M., Stern, S., Nass, K., Andritschke, R., Schröter, C.-D., Krasniqi, F., Bott, M., Schmidt, K. E., Wang, X., Grotjohann, I., Holton, J. M., Barends, T. R. M., Neutze, R., Marchesini, S., Fromme, R., Schorb, S., Rupp, D., Adolph, M., Gorkhover, T., Andersson, I., Hirsemann, H., Potdevin, G., Graafsma, H., Nilsson, B. & Spence, J. C. H. (2011). *Nature*, **470**, 73–77.

Choo, Y.-J. & Kang, B.-S. (2002). *Phys. Fluids*, **14**, 622–627.

DePonte, D. P., Weierstall, U., Schmidt, K., Warner, J., Starodub, D., Spence, J. C. H. & Doak, R. B. (2008). *J. Phys. D Appl. Phys.* **41**, 195505.

Eggers, J. & Villermaux, E. (2008). *Rep. Prog. Phys.* **71**, 036601.

Ekimova, M., Quevedo, W., Faubel, M., Wernet, P. & Nibbering, E. T. J. (2015). *Struct. Dyn.* **2**, 054301.

Fondell, M., Eckert, S., Jay, R. M., Weniger, C., Quevedo, W., Niskanen, J., Kennedy, B., Sorgenfrei, F., Schick, D., Giangrisostomi, E., Ovsyannikov, R., Adamczyk, K., Huse, N., Wernet, P., Mitzner, R. & Föhlisch, A. (2017). *Struct. Dyn.* **4**, 054902.

Gañán-Calvo, A. M. (1998). *Phys. Rev. Lett.* **80**, 285–288.

George, K. M., Morrison, J. T., Feister, S., Ngirmang, G. K., Smith, J. R., Klim, A. J., Snyder, J., Austin, D., Erbsen, W., Frische, K. D., Nees, J., Orban, C., Chowdhury, E. A. & Roquemore, W. M. (2019). *High Power Laser Sci. Eng.*, **7**, e50.

Grünbein, M. L., Bielecki, J., Gorel, A., Stricker, M., Bean, R., Cammarata, M., Dörner, K., Fröhlich, L., Hartmann, E., Hauf, S., Hilpert, M., Kim, Y., Kloos, M., Letrun, R., Messerschmidt, M., Mills, G., Nass Kovacs, G., Ramilli, M., Roome, C. M., Sato, T., Scholz, M., Sliwa, M., Sztuk-Dambietz, J., Weik, M., Weinhausen, B., Al-Qudami, N., Boukhelef, D., Brockhauser, S., Ehsan, W., Emons, M., Esenov, S., Fangohr, H., Kaukher, A., Kluyver, T., Lederer, M., Maia, L., Manetti, M., Michelat, T., Münnich, A., Pallas, F., Palmer, G., Previtali, G., Raab, N., Silenzi, A., Szuba, J., Venkatesan, S., Wrona, K., Zhu, J., Doak, R. B., Shoeman, R. L., Foucar, L., Colletier, J.-P., Mancuso, A. P., Barends, T. R. M., Stan, C. A. & Schlichting, I. (2018). *Nat. Commun.* **9**, 3487.

Ha, B., DePonte, D. P. & Santiago, J. G. (2018). *Phys. Rev. Fluids*, **3**, 114202.

Hoffman, D. J., Bechtel, H. A., Huyke, D. A., Santiago, J. G., DePonte, D. P. & Koralek, J. D. (2022*a*). *Langmuir*, **38**, 12822–12832.

Hoffman, D. J., Van Driel, T. B., Kroll, T., Crissman, C. J., Ryland, E. S., Nelson, K. J., Cordones, A. A., Koralek, J. D. & DePonte, D. P. (2022*b*). *Front. Mol. Biosci.* **9**, 1048932.

Klebl, D. P., Gravett, M. S. C., Kontziampasis, D., Wright, D. J., Bon, R. S., Monteiro, D. C. F., Trebbin, M., Sobott, F., White, H. D., Darrow, M. C., Thompson, R. F. & Muench, S. P. (2020*a*). *Structure*, **28**, 1238–1248.e4.

Klebl, D. P., Monteiro, D. C. F., Kontziampasis, D., Kopf, F., Sobott, F., White, H. D., Trebbin, M. & Muench, S. P. (2020*b*). *Acta Cryst.* D**76**, 340–349.

Knoška, J., Adriano, L., Awel, S., Beyerlein, K. R., Yefanov, O., Oberthuer, D., Peña Murillo, G. E., Roth, N., Sarrou, I., Villanueva-Perez, P., Wiedorn, M. O., Wilde, F., Bajt, S., Chapman, H. N. & Heymann, M. (2020).

Nat. Commun. **11**, 657.

Konold, P. E., You, T., Bielecki, J., Valerio, J., Kloos, M., Westphal, D., Bellisario, A., Varma Yenupuri, T., Wollter, A., Koliyadu, J. C. P., Koua, F. H. M., Letrun, R., Round, A., Sato, T., Mészáros, P., Monrroy, L., Mutisya, J., Bódizs, S., Larkiala, T., Nimmrich, A., Alvarez, R., Adams, P., Bean, R., Ekeberg, T., Kirian, R. A., Martin, A. V., Westenhoff, S. & Maia, F. R. N. C. (2023). *IUCrJ*, **10**, 662–670.

Kontziampasis, D., Klebl, D. P., Iadanza, M. G., Scarff, C. A., Kopf, F., Sobott, F., Monteiro, D. C. F., Trebbin, M., Muench, S. P. & White, H. D. (2019). *IUCrJ*, **6**, 1024–1031.

Koralek, J. D., Kim, J. B., Brůža, P., Curry, C. B., Chen, Z., Bechtel, H. A., Cordones, A. A., Sperling, P., Toleikis, S., Kern, J. F., Moeller, S. P., Glenzer, S. H. & DePonte, D. P. (2018). *Nat. Commun.* **9**, 1353.

Kraus, P. M., Zürch, M., Cushing, S. K., Neumark, D. M. & Leone, S. R. (2018). *Nat. Rev. Chem.* **2**, 82–94.

Kurta, R. P., Donatelli, J. J., Yoon, C. H., Berntsen, P., Bielecki, J., Daurer, B. J., DeMirci, H., Fromme, P., Hantke, M. F., Maia, F. R. N. C., Munke, A., Nettelblad, C., Pande, K., Reddy, H. K. N., Sellberg, J. A., Sierra, R. G., Svenda, M., van der Schot, G., Vartanyants, I. A., Williams, G. J., Xavier, P. L., Aquila, A., Zwart, P. H. & Mancuso, A. P. (2017). *Phys. Rev. Lett.* **119**, 158102.

Luu, T. T., Yin, Z., Jain, A., Gaumnitz, T., Pertot, Y., Ma, J. & Wörner, H. J. (2018). *Nat. Commun.* **9**, 3723.

Nazari, R., Zaare, S., Alvarez, R. C., Karpos, K., Engelman, T., Madsen, C., Nelson, G., Spence, J. C. H., Weierstall, U., Adrian, R. J. & Kirian, R. A. (2020). *Opt. Express*, **28**, 21749–21765.

Nelson, G., Kirian, R. A., Weierstall, U., Zatsepin, N. A., Faragó, T., Baumbach, T., Wilde, F., Niesler, F. B. P., Zimmer, B., Ishigami, I., Hikita, M., Bajt, S., Yeh, S.-R., Rousseau, D. L., Chapman, H. N., Spence, J. C. H. & Heymann, M. (2016). *Opt. Express*, **24**, 11515–11530.

Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. & Hajdu, J. (2000). *Nature*, **406**, 752–757.

Nunes, J. P. F., Ledbetter, K., Lin, M., Kozina, M., DePonte, D. P., Biasin, E., Centurion, M., Crissman, C. J., Dunning, M., Guillet, S., Jobe, K., Liu, Y., Mo, M., Shen, X., Sublett, R., Weathersby, S., Yoneda, C., Wolf, T. J. A., Yang, J., Cordones, A. A. & Wang, X. J. (2020). *Struct. Dyn.* **7**, 024301.

Oberthuer, D., Knoška, J., Wiedorn, M. O., Beyerlein, K. R., Bushnell, D. A., Kovaleva, E. G., Heymann, M., Gumprecht, L., Kirian, R. A., Barty, A., Mariani, V., Tolstikova, A., Adriano, L., Awel, S., Barthelmess, M., Dörner, K., Xavier, P. L., Yefanov, O., James, D. R., Nelson, G., Wang, D., Calvey, G., Chen, Y., Schmidt, A., Szczepek, M., Frielingsdorf, S., Lenz, O., Snell, E., Robinson, P. J., Šarler, B., Belšak, G., Maček, M., Wilde, F., Aquila, A., Boutet, S., Liang, M., Hunter, M. S., Scheerer, P., Lipscomb, J. D., Weierstall, U., Kornberg, R. D., Spence, J. C. H., Pollack, L., Chapman, H. N. & Bajt, S. (2017). *Sci. Rep.* **7**, 44628.

Pande, K., Donatelli, J. J., Malmerberg, E., Foucar, L., Bostedt, C., Schlichting, I. & Zwart, P. H. (2018). *Proc. Natl Acad. Sci. USA*, **115**, 11772–11777.

Smith, A. D., Balčiūnas, T., Chang, Y.-P., Schmidt, C., Zinchenko, K., Nunes, F. B., Rossi, E., Svoboda, V., Yin, Z., Wolf, J.-P. & Wörner, H. J. (2020). *J. Phys. Chem. Lett.* **11**, 1981–1988.

Sobolev, E., Zolotarev, S., Giewekemeyer, K., Bielecki, J., Okamoto, K., Reddy, H. K. N., Andreasson, J., Ayyer, K., Barak, I., Bari, S., Barty, A., Bean, R., Bobkov, S., Chapman, H. N., Chojnowski, G., Daurer, B. J., Dörner, K., Ekeberg, T., Flückiger, L., Galzitskaya, O., Gelisio, L., Hauf, S., Hogue, B. G., Horke, D. A., Hosseinizadeh, A., Ilyin, V., Jung, C., Kim, C., Kim, Y., Kirian, R. A., Kirkwood, H., Kulyk, O., Küpper, J.,

Letrun, R., Loh, N. D., Lorenzen, K., Messerschmidt, M., Mühlig, K., Ourmazd, A., Raab, N., Rode, A. V., Rose, M., Round, A., Sato, T., Schubert, R., Schwander, P., Sellberg, J. A., Sikorski, M., Silenzi, A., Song, C., Spence, J. C. H., Stern, S., Sztuk-Dambietz, J., Teslyuk, A., Timneanu, N., Trebbin, M., Uetrecht, C., Weinhausen, B., Williams, G. J., Xavier, P. L., Xu, C., Vartanyants, I. A., Lamzin, V. S., Mancuso, A. & Maia, F. R. N. C. (2020). *Commun. Phys.* **3**, 97.

Stan, C. A., Milathianaki, D., Laksmono, H., Sierra, R. G., McQueen, T. A., Messerschmidt, M., Williams, G. J., Koglin, J. E., Lane, T. J., Hayes, M. J., Guillet, S. A. H., Liang, M., Aquila, A. L., Willmott, P. R., Robinson, J. S., Gumerlock, K. L., Botha, S., Nass, K., Schlichting, I., Shoeman, R. L., Stone, H. A. & Boutet, S. (2016). *Nat. Phys.* **12**, 966–971.

Taylor, G. (1960). *Proc. R. Soc. London Ser. A*, **259**, 1–17.

Trebbin, M., Krüger, K., DePonte, D., Roth, S. V., Chapman, H. N. & Förster, S. (2014). *Lab Chip*, **14**, 1733–1745.

Vakili, M., Vasireddi, R., Gwozdz, P. V., Monteiro, D. C. F., Heymann, M., Blick, R. H. & Trebbin, M. (2020). *Rev. Sci. Instrum.* **91**, 085108.

Vakili, M., Bielecki, J., Knoška, J., Otte, F., Han, H., Kloos, M., Schubert, R., Delmas, E., Mills, G., de Wijn, R., Letrun, R., Dold, S., Bean, R., Round, A., Kim, Y., Lima, F. A., Dörner, K., Valerio, J., Heymann, M., Mancuso, A. P. & Schulz, J. (2022). *J. Synchrotron Rad.* **29**, 331–346.

Wiedorn, M. O., Awel, S., Morgan, A. J., Ayyer, K., Gevorkov, Y., Fleckenstein, H., Roth, N., Adriano, L., Bean, R., Beyerlein, K. R., Chen, J., Coe, J., Cruz-Mazo, F., Ekeberg, T., Graceffa, R., Heymann, M., Horke, D. A., Knoška, J., Mariani, V., Nazari, R., Oberthür, D., Samanta, A. K., Sierra, R. G., Stan, C. A., Yefanov, O., Rompotis, D., Correa, J., Erk, B., Treusch, R., Schulz, J., Hogue, B. G., Gañán-Calvo, A. M., Fromme, P., Küpper, J., Rode, A. V., Bajt, S., Kirian, R. A. & Chapman, H. N. (2018*a*). *IUCrJ*, **5**, 574–584.

Wiedorn, M. O., Oberthür, D., Bean, R., Schubert, R., Werner, N., Abbey, B., Aepfelbacher, M., Adriano, L., Allahgholi, A., Al-Qudami, N., Andreasson, J., Aplin, S., Awel, S., Ayyer, K., Bajt, S., Barák, I., Bari, S., Bielecki, J., Botha, S., Boukhelef, D., Brehm, W., Brockhauser, S., Cheviakov, I., Coleman, M. A., Cruz-Mazo, F., Danilevski, C., Darmanin, C., Doak, R. B., Domaracky, M., Dörner, K., Du, Y., Fangohr, H., Fleckenstein, H., Frank, M., Fromme, P., Gañán-Calvo, A. M., Gevorkov, Y., Giewekemeyer, K., Ginn, H. M., Graafsma, H., Graceffa, R., Greiffenberg, D., Gumprecht, L., Göttlicher, P., Hajdu, J., Hauf, S., Heymann, M., Holmes, S., Horke, D. A., Hunter, M. S., Imlau, S., Kaukher, A., Kim, Y., Klyuev, A., Knoška, J., Kobe, B., Kuhn, M., Kupitz, C., Küpper, J., Lahey-Rudolph, J. M., Laurus, T., Le Cong, K., Letrun, R., Xavier, P. L., Maia, L., Maia, F. R. N. C., Mariani, V., Messerschmidt, M., Metz, M., Mezza, D., Michelat, T., Mills, G., Monteiro, D. C. F., Morgan, A., Mühlig, K., Munke, A., Münnich, A., Nette, J., Nugent, K. A., Nuguid, T., Orville, A. M., Pandey, S., Pena, G., Villanueva-Perez, P., Poehlsen, J., Previtali, G., Redecke, L., Riekehr, W. M., Rohde, H., Round, A., Safenreiter, T., Sarrou, I., Sato, T., Schmidt, M., Schmitt, B., Schönherr, R., Schulz, J., Sellberg, J. A., Seibert, M. M., Seuring, C., Shelby, M. L., Shoeman, R. L., Sikorski, M., Silenzi, A., Stan, C. A., Shi, X., Stern, S., Sztuk-Dambietz, J., Szuba, J., Tolstikova, A., Trebbin, M., Trunk, U., Vagovic, P., Ve, T., Weinhausen, B., White, T. A., Wrona, K., Xu, C., Yefanov, O., Zatsepin, N., Zhang, J., Perbandt, M., Mancuso, A. P., Betzel, C., Chapman, H. & Barty, A. (2018*b*). *Nat. Commun.* **9**, 4025.

Yang, J., Nunes, J. P. F., Ledbetter, K., Biasin, E., Centurion, M., Chen, Z., Cordones, A. A., Crissman, C., Deponte, D. P., Glenzer, S. H., Lin, M.-F., Mo, M., Rankine, C. D., Shen, X., Wolf, T. J. A. & Wang, X. (2021). *Phys. Chem. Chem. Phys.* **23**, 1308–1316.

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IUCR CONGRESS

Crystal-a-con at IUCr2023



Bragg Your Pattern competition winners' art was displayed on our Giant Buckyball. Photo of the buckyball: S. R. Batten.

Stuart R. Batten, Helen E. Maynard-Casely, Rosemary J. Young, Emily J. Furlong, Bryce G. Mullens

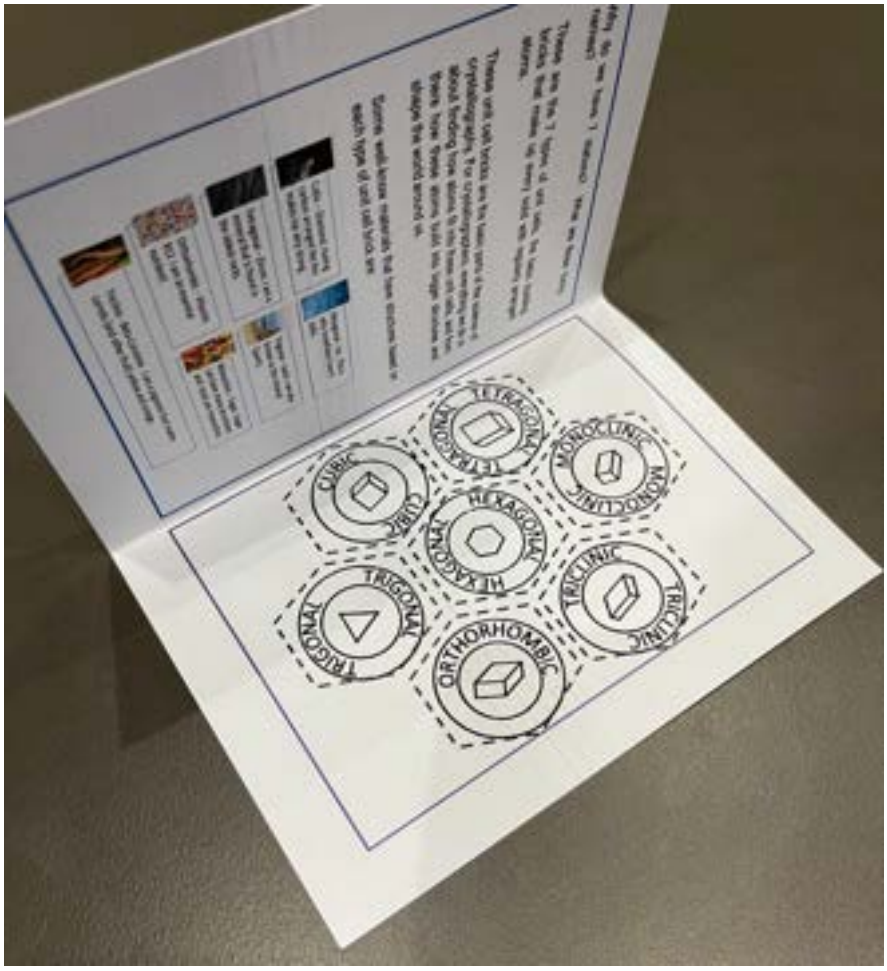
How many times in your career have the world’s crystallographers gathered in your town (or even your country when you are in the Southern Hemisphere)? From the point that the SCANZ team won the bid to hold the 26th IUCr Congress in Melbourne, we realised that this was truly a once-in-a-lifetime opportunity to push communication of crystallography beyond the Brillouin zone. And so, the Bragg Your Pattern project (https://braggyourpattern.com) was formed!



The Bragg Your Pattern committee proudly wearing the popular Bragg T-shirts specially commissioned for the conference (available still from https://meganleestudio.com/). Photo: IUCr2023 Congress.

In Australia and New Zealand, there is a big emphasis on developing science, technology, engineering and mathematics (STEM) resources for students in high schools (aged 11 and above) but less on those younger. The Bragg Your Pattern team realised that, through patterns and symmetry and its very visual nature, crystallography is an ideal topic to target with a younger audience. We started the project in 2022 with a national pattern competition, where students were encouraged to ‘make’ or ‘see’ a pattern and send the image to us. Those who made it to IUCr2023 would have seen these images on our Giant Buckyball during the conference.

But the pattern competition was just our warm-up, with the big event planned for 2023 – a pop-up crystallographic science festival held right within the conference venue! We brought together crystallographic-inspired exhibits, but our big draw was the inclusion of seven interactive activities. The event – ‘Crystal-a-con’ – was marketed to schools and members of the public and held on Friday and Saturday during the congress. Each of the interactive activities was named after a crystal system, and each visitor was given a passport so that they could collect stamps from each one.



A completed Crystal-a-con passport. Photo: R. J. Young.

Our **Cubic** activity was perhaps our headline activity, and certainly the one that attracted many IUCr delegates – trying to break the world record for the largest crystal structure model! The previous record (https://guinnessworldrecords.com/world-records/109929-largest-sodium-chloride-molecular-structure-model) was for a model of sodium chloride (common table salt), which contained 38,880 individual ‘atoms’ (though it has since been expanded to 42,875 atoms, https://worldrecord.r-krickl.com/en/, https://www.facebook.com/worldrecordcrystalmodel).

In the weeks before the conference started, a number of smaller parts of the overall model were built by staff at the Australian Synchrotron. These pre-built parts were taken to the conference venue and assembled and added to by conference delegates over the first five days of the conference. School groups and members of the public who attended Crystal-a-con also helped build the big model.



The world-record diamond attempt proved a popular networking spot for delegates of IUCr2023, as well as a big draw as an interactive activity during Crystal-a-con. Photo: Thomas Proffen.

The statistics of the final assembled model were impressive: 62,356 atoms were connected by 121,547 bonds (*i.e.* 183,903 individual components that had to be connected together), total weight 341 kg, total volume 4.47 m^3. The dimensions were 3.69 m along the bottom triangular edges, 2.31 m along the top triangular edges, and 1.11 m in height.



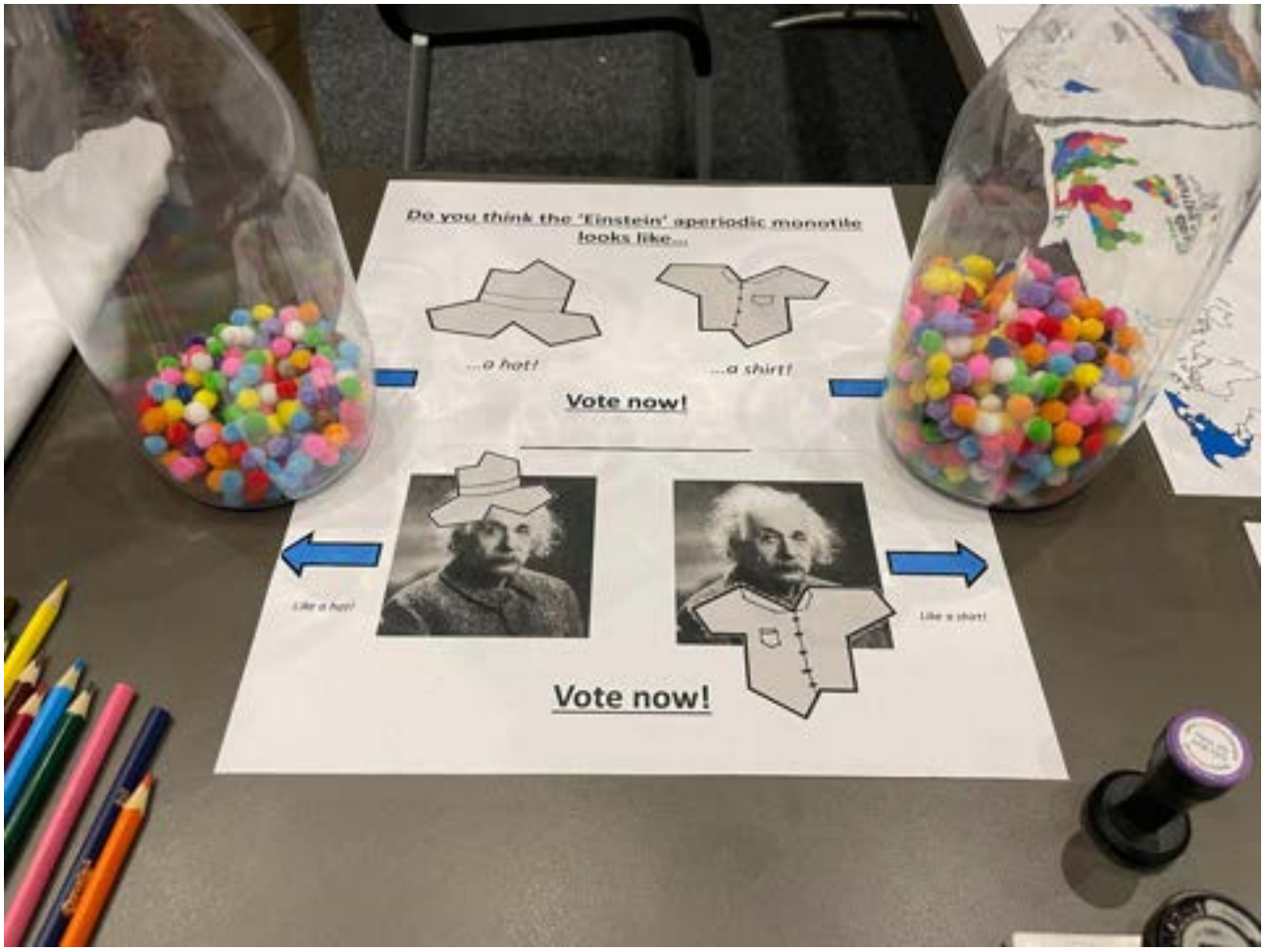
The completed world-record diamond model. Photo: S. R. Batten.

Our **Hexagonal** activity was on the sweet side! Sweets and crystals are both amazing individually but together they are the best! Participants in the hexagonal activity built their own crystal structure models out of jubes (Australian jelly sweets) and toothpicks, using over 25 kg of lollies and 10,000 toothpicks. Starting with a simple cubic crystal structure, it was quickly apparent that this model was quite brittle and weak. Adding another lolly to make a body-centred cubic structure made a much stronger assembly. Enthusiastic kids continued on to make extended body-centred cubic and hexagonal structures.

This activity was an excellent conversation starter to talk about everyday crystals such as salt and sugar and how they are similar to and different from crystals like diamonds and rubies. The different ways the same building blocks (jubes and toothpicks) could be constructed to make stronger or weaker assemblies could be directly related to the difference between diamonds and graphite.

Many kids worked together to combine their ‘unit cells’ to make larger and larger lolly ‘crystallites’, even making them colour-coordinated. This activity was very popular, although that may have been because they could eat their lollies after they finished building!

Celebrating the patterns of the world was the theme for the **Trigonal** activity, which brought together a range of patterns from different cultures and explored the maths behind them (with Dr Katherine Seaton). Not only were participants able to create their own inspired patterns, but we also got them thinking “When is a pattern not a pattern?” by introducing the ‘Einstein’ shape that had taken the news by storm a few months previously. Visitors were also encouraged to vote if they thought the shape most resembled a hat or a shirt! As you can see in the picture, the shirt won!



Hat or shirt? Crystal-a-con visitors were able to vote on what they thought the latest Einstein shape most looked like. Photo: H. E. Maynard-Casely.

Our **Orthorhombic** and **Tetrahedral** activities were run by some fantastic partners. The CCDC brought their 'Crystal detectives' (https://www.ccdc.cam.ac.uk/community/education-and-outreach/outreach/home-learning-activities/identikit-of-common-substances/) activity that they had run at a number of science festivals. The Australian audience had a great time identifying common substances from crystal structures; through the link, anyone can try this at home too. Added to this, ANSTO – custodians of the central facilities in Australia – dispatched a team from their Discovery Centre to run a diffraction demonstrating activity with lasers on the Friday, while the Saturday theme revolved around the periodic table.

In the **Monoclinic** activity, the Crystal-a-con participants had the opportunity to build their own virus model out of paper! Thanks to the RCSB Protein Data Bank, we had a very nice template that could be easily punched out of a piece of card and folded up to make a Zika virus model. For those participants wanting more of a challenge, Protein Data Bank Japan provided instructions and paper to fold an origami virus, and Dr Daniel Eriksson was on hand to help people fold an icosahedral virus from a single piece of paper. The Protein Data Bank in Europe was also involved and provided beautiful images from their 2023 PDB art calendar to display.

Our **Triclinic** or 'Meet the Crystallographer' station allowed us to make the most of the amazing crystallographers who had travelled from the other side of the world to attend IUCr2023. We had 12 crystallographers volunteer to share their work with our participants over the 1.5 days. These crystallographers came from countries across the globe, including the UK, Uruguay, Germany, Canada and, of course, Australia. The Crystal-a-con participants were amazed to hear about all the fascinating work the crystallographers do and were excited to take home Professor Jennifer Martin's *My Aunt is a Protein Crystal Scientist* book and goodies from the Diamond Synchrotron.



A big thanks goes to all who helped make Crystal-a-con a reality, including many staff at the Australian Synchrotron who provided invaluable support for the logistics. Photo: H. E. Maynard-Casely.

Along with the interactive activities, we gathered together a number of additional exhibits, from crystallographic-inspired fashion (thanks to Dr Irene Suarez-Martinez with her Stem and Needles project, https://stemandneedles.com/) to giant crystal structures that had first been commissioned for the International Year of Crystallography in 2014. Overall we created a pop-up science museum!



The knitted neuraminidase – one of our giant crystal structures from 2014. Photo: R. J. Young.

As the icing on the cake, we organized a public lecture by Professor Jenny Martin, who shared why she loves crystallography. The lecture touched on Australia's strong connection to this wonderful science, the incredible women who work in the field, and the amazing scientific advances our community has enabled through sharing resources and knowledge.



Professor Jenny Martin signing copies of *My Aunt is a Protein Crystal Scientist* after her public lecture. Photo: R. J. Young.

A big thanks goes to all who helped to make the event the success it was: our IUCr volunteers (sporting their red Bragg T-shirts), the synchrotron staff who tirelessly made the diamond model and were invaluable in the logistics, and the conference organisers who supported the whole endeavour. Thanks also to all the IUCr delegates who stopped by and put some carbon atoms together; the event was truly community-supported.

Overall, our Crystal-a-con event was visited by 480 school kids, teachers and their families, giving them a great insight into the importance of crystallography and what life looks like on the atomic scale.

What are our next steps? Our giant diamond model is now destined to be broken down into individual kits and will be donated, along with a supporting booklet, to more than 1000 primary schools all over Australia and New Zealand to inspire the next generation of scientists and crystallographers. Particular emphasis will be given to remote, rural, regional and low-economic-opportunity schools, which are typically under-resourced in the area of STEM and/or have limited access due to their distance from other STEM-supporting outreach programmes. Hopefully, this, and the fact that we now have a toolkit of activities to run around the country, will mean a long public outreach legacy for the IUCr2023 meeting.

MEETING REPORT (IUCR SUPPORTED)

73rd Annual Meeting of the ACA: The Structural Science Society (ACA2023)



Anna Gardberg, Samantha Powell

The 73rd Annual Meeting of the American Crystallographic Association: The Structural Science Society was held in Baltimore, MD, USA, on the traditional ancestral lands of the Piscataway and the Susquehannock tribes. At both the opening and the closing of the meeting, we respectfully acknowledged and honored all indigenous communities – past, present and future.

The scientific program spanned 8–11 July 2023, with associated workshops on 7 July. The program consisted of 47 daytime scientific sessions, 2 evening sessions, 3 poster sessions, 5 workshops and a 3-minute thesis competition. In contrast to ACA2022, this meeting was offered entirely in-person. The meeting was well-attended, with over 500 registrants and over 160 workshop participants.

The scientific program opened with a keynote address from Sir Venki Ramakrishnan, whose lecture 'My Adventures in the Ribosome' was a wide-ranging overview of his personal and professional journey, culminating in unraveling the ribosome’s structure, and concluding by relaying how newer structural methods such as cryo-electron microscopy (cryoEM) are enabling us to tackle ever-harder structural problems. Expanding on that theme, the Transactions Symposium was entitled 'From Atoms to Cells – Electron Microscopy for Structure Solution'. The subsequent 3 days continued with 6 parallel tracks of scientific sessions as well as 3 poster sessions.



Other highlights of the meeting were the sessions on machine learning, AI and related subjects that are very topical to our profession. As well, the evening 'Would you publish this?' session featured both small-molecule and macromolecular entries, filled the venue and proved one of the most convivial of the week.

This year’s program continued to demonstrate the relevance of our new name, ACA: The Structural Science Society. We saw many talks covering structural techniques outside of traditional crystallography, such as BioSAXS and SANS, and multi-modal experiments. Sessions on cryoEM and related techniques such as cryo-electron tomography (cryoET) and microcrystal electron diffraction (MicroED) were also prominent, being featured in the Transactions Symposium as well as 5 other sessions.

Details on this and future meetings can be found here. More information can be found on our social media accounts on X and Instagram @ACAxtal, Facebook @AmerCrystalAssn or LinkedIn. In anticipation of an in-person meeting for 2024, please mark your calendars to join us on 7–11 July 2024 in Denver, CO!

MEETING REPORT

11th Training course on symmetry and group theory



Group photo of the 2023 Japanese basic course.

Noriyuki Igarashi

The training course on symmetry and group theory in Japan was launched in August 2014, immediately after the IUCr Congress in Montreal, on the occasion of the International Year of Crystallography. The motivation was to compensate for the lack for basic crystallography training in university curricula, which results in serious obstacles in daily crystallographic work when the investigator needs to interpret their results, navigate through the *International Tables for Crystallography* and perform all the tasks that a black box cannot do for them.

The training course is hosted at the High Energy Accelerator Organization site in Tsukuba and is offered free of charge to all students and scientists in Japan who need basic training in crystallographic symmetry. It is sponsored by the Crystallographic Society of Japan and the Institute of Materials Structure Science of the High Energy Accelerator Organization, and supported by a number of Japanese scientific societies and associations. It benefits from the precious help of Ms Yoshimi Takahashi, the dedicated secretary in charge of all the logistics and contact with participants.

The course spans five full days, with morning and afternoon lectures and exercises, and night sessions for questions and answers, discussion and support for the exercises. It is taught in its entirety by Professor Massimo Nespolo, from the Université de Lorraine (France). The unexpected success of the first course convinced the organizers to repeat it twice a year (March, August) until 2017, moving then to a once-a-year frequency when it became an official Interdisciplinary Lecture of the Graduate University for Advanced Studies (Sokendai), which entered as co-sponsor. This year it was held in July.

The programme of the training course starts from basic algebra to bring everybody to a common background, and goes through theory and practice of crystallographic point and space groups, with extensive exercises on the *International Tables for Crystallography*, crystallographic calculations, group–subgroup relations, normalizers, chirality, geometric derivation of reflection conditions, crystallographic orbits and symmetry aspects of phase transitions, with examples of derivative structures and construction of a structural model of low-symmetry polymorphs from high-symmetry polymorphs.

The course is taught entirely in Japanese. Because of the language difficulties met by foreign students willing to attend the lectures, an English version has been offered since 2019, but had to be interrupted because of the SARS-CoV-2 outbreak in 2020 and could only be restarted this year, after foreign students were again allowed to come and study in Japan. The Japanese course was only suspended in 2020; in

2021 it was offered in a hybrid form, before going back to on-site lectures in 2022.



Group photo of the 2023 English basic course.

An advanced course is offered periodically to those who have attended the basic course. The first advanced course was offered in 2016. The second advanced course, originally planned for 2020–2021, had to be postponed and was eventually realized this year, with a programme centred on groupoids and chromatic symmetry.



Group photo of the 2023 advanced course.

The 12th course is planned for July 2024, both in English and Japanese.

Professor Noriyuki Igarashi (KEK, Tsukuba) is Chair of the Local Organizing Committee of the training course.

MEETING REPORT (IUCR SUPPORTED)

Electron Crystallography School 2023



Laure Bourgeois, Hongyi Xu, Tatiana Gorelik

On 19–21 August 2023, the Monash Centre for Electron Microscopy (MCEM) hosted the Electron Crystallography School 2023 (ECS2023) as a satellite event to the 26th IUCr Congress. The School was organised by the IUCr Commission on Electron Crystallography, with Hongyi Xu, Tatiana Gorelik, Mauro Gemmi and Laure Bourgeois as co-chairs.

The ECS2023 focused on two broad topics that have seen considerable development in the last decade or so: 4D scanning transmission electron microscopy (4D-STEM) and 3D/micro-electron diffraction (3D-ED). These developments have led to major advances in the characterisation of the atomic-scale structure of solid matter, from energy materials and green chemicals to glasses, proteins and pharmaceutical compounds.

The School was aimed at postgraduate students, early-career researchers and newcomers to the field. It offered a series of lectures on the fundamental theory underpinning 4D-STEM and 3D-ED, together with historical background, software demonstrations and hands-on tutorials. The intensive program also included a live demonstration on MCEM’s latest transmission electron microscope acquisition, the Thermo Fisher Scientific Spectra-φ. A session was dedicated to presentations from industry scientists. There was also a lively poster session and a tour of MCEM facilities.



ECS2023 included presentations from many distinguished international scientists including Professor Lukáš Palatinus from the Czech Academy of Sciences, shown here.

The School was very fortunate to have 20 distinguished scientists from both overseas and Australia as its speakers. Amongst them were Ute Kolb (Johannes Gutenberg Universität Mainz) and Jian-Min Zuo (University of Illinois), past and present recipients of the Gjønnes Medal in Electron Crystallography, the highest distinction in the field.

Over 70 delegates from 13 countries and 4 continents attended the School, with students and researchers from countries as far away as Brazil, Belgium and China. This included a significant cohort from the X-ray crystallography community. Feedback from attendees was very positive, with appreciation shown not only for the quality of the program but also for the opportunity to meet with the broad crystallography community.

The organising committee is grateful for the generous support from the following sponsors: the IUCr, Microscopy Australia, the Society of Crystallographers in Australia and New Zealand (SCANZ), Rigaku, JEOL, Thermo Fisher Scientific, Dectris, ReadCrystal, Gatan Ametek and NanoMEGAS. The IUCr grants supported 13 PhD students and postdoctoral researchers, 4 of whom came from overseas (Belgium, Germany and China).

More detail can be found on the ECS2023 website.

Reports from IUCr grant recipients

Loreibelle Abian, Monash University, Australia

This student recipient was given the opportunity to attend the Electron Crystallography School 2023 last 19–21 August 2023 at Monash University-Clayton Campus, Clayton, Victoria, Australia. The said endeavour was attended by postgraduate students and early-career researchers coming from different countries as well as remarkable presenters from diverse fields of electron crystallography. The invited speakers talked about the advances in electron crystallography and cutting-edge technologies behind the state-of-the art instruments used in electron microscopy. The 3-day activity enabled the student to widen her horizon in the area of electron diffraction as she learned about other electron microscopy methods aside from the convergent-beam electron diffraction (CBED) technique which she currently employs in her research in investigating chemical bonding in inhomogeneous materials. The discussions during the lectures tackled CBED, scanning electron nanodiffraction (SEND), 4D scanning transmission electron microscopy (4D-STEM), 3D electron diffraction (3D-ED) and micro-electron diffraction (MicroED). The presentations were excellently delivered in that they undertook not only the fundamentals in crystallography and microscopy but also the latest research into which a speaker’s group is involved. Moreover, the participants were provided with a platform to share their research during the poster presentation on the evening of the first day where they were able to acquire insights and recommendations from renowned scientists and experts who graced the said event. The student would like to extend her gratitude for the sponsorship to join ECS which has given her an avenue to learn more about her research and to connect and build networks with fellow researchers.

Bikas Aryal, Monash University, Australia

The Electron Crystallography School (ECS) held at Monash University provided the attendees with both theoretical concepts of electron diffraction through excellent lectures and practical concepts through live software and TEM operation demonstrations. The ECS covered a wide range of topics related to electron diffraction and crystallography, such as selected area electron diffraction (SAED), scanning electron nanodiffraction (SEND), scanning transmission electron microscopy (STEM), quantitative convergent-beam electron diffraction (QCBED), MicroED, ptychography and 4D-STEM. By participating in ECS, I got a chance to understand the fundamentals of electron diffraction and advances in different techniques like 4D-STEM, SEND, MicroED and ptychography. As my research focuses on chemical bonding studies using QCBED, I enjoyed the talks “Direct observation of *d*-holes in Cu_2O” and “Measuring vacancy concentrations, chemical bonding and lattice contraction around nanovoids in aluminium by QCBED”.

Furthermore, the ECS provided me with an opportunity to meet world-renowned experts such as Jian-Min Zuo, Randi Holmestad, Lukáš Palatinus, Ute Kolb and Colin Ophus. I discussed future collaborations with Professor Zuo. I also met many early-career researchers and representatives from different companies. We discussed new research directions and explored industrial collaborations.

I am grateful for the International Union of Crystallography's (IUCr) financial assistance, which greatly aided in covering my travel costs. The main benefit of these scholarships is their capacity to open up educational opportunities and scientific events to a wide range of participants.

Wei Chao, Monash University, Australia

I am so honoured and grateful for being selected as a recipient of an IUCr grant, which has allowed me to participate in the Electron Crystallography School. The school seamlessly integrated applications of electron diffraction in both materials science and biology, providing me with a highly educational and inspirational experience. This unique opportunity has enabled me to engage with presentations by pioneers in convergent-beam electron diffraction, 3D-ED/MicroED, offering invaluable insights into the beauty of diffraction across diverse disciplines.

The content of the school was so well organized. As a researcher in materials science, I not only enjoyed outstanding talks within my field but also had the chance to explore a new area of study. Despite my limited knowledge of MicroED, I learned and enjoyed a lot from the well-structured and comprehensive talks. I am sure that students and young researchers in the MicroED field would similarly find value in the discussions on convergent-beam electron diffraction.

The inclusion of hands-on workshops, focused on software packages, added a practical dimension that I found particularly enriching.

I would like to express my sincere gratitude to the organizers for their dedicated efforts in making this event a success. It is such a valuable experience in my career. I also wish to express my deep appreciation to the committee for the grant, which makes my attendance at this wonderful event possible.

Mostafa Eid Abdelmaboud Ahmed Ali, Monash University, Australia

The Electron Crystallography School (ECS), held between 19 and 21 August 2023 at Monash University, aimed to expand our knowledge of the electron crystallography area and provided us with a unique platform to explore it. The ECS covered a wide range of topics, providing attendees with both theoretical information through excellent lectures and practical skills through software demonstrations. For example, the lectures covered fundamental principles of electron crystallography techniques such as selected area electron diffraction (SAED), scanning electron nanodiffraction (SEND), scanning transmission electron microscopy (STEM), convergent-beam electron diffraction (CBED), quantitative convergent-beam electron diffraction (QCBED) and 4D-STEM.

Furthermore, the lectures and hands-on sessions (software demos) were presented by renowned experts and academics from top universities around the world, ensuring a thorough understanding of the subject matter. For example, Professor Jian-Min Zuo, a pioneer and brilliant in the field of electron crystallography, was among those present. I met him at the school, introduced myself and my proposal to him, and discussed some electron diffraction topics with him. This was very much appreciated.

My PhD research focuses on CBED and QCBED approaches, therefore I really learned a lot about the current issues and applications surrounding these methods, as well as the difficulties in gathering and interpreting electron diffraction data and ways to get over these obstacles. For instance, as one of the QCBED applications, I was interested in Professor Zuo's lecture “Direct observation of *d*-holes in Cu_2O” and Professor Philip Nakashima's session “Vacancy mapping in Al structure”.

Besides the mentioned benefits of attending ECS, I was very happy for the International Union of Crystallography (IUCr) financial support, which helped me a lot to cover travel expenses. The primary impact of such grants lies in their ability to make educational opportunities and scientific events accessible to a diverse range of participants.

Weilun Li, Monash University, Australia

Overview

The Electron Crystallography School proved to be an enriching experience, offering a comprehensive understanding of advanced techniques in structural analysis using electron crystallography. Held at Monash, Melbourne, the school gathered a diverse group of researchers, scientists and students eager to delve into the intricacies of this cutting-edge field.

Programs and lectures

The school commenced with insightful lectures by eminent speakers who shared their expertise on the theoretical foundations of electron crystallography, its applications and recent advancements in the field. These lectures provided a solid foundation for participants, irrespective of their prior knowledge, ensuring that everyone could grasp the complexities of electron crystallography. The combination of CBED and 4D-STEM on the first day and 3D-ED and MicroED on the following day proved to be extremely effective.

Hands-on sessions

A highlight of the Electron Crystallography School was the demo lab sessions on the state-of-the-art TEM at Monash Centre for Electron Microscopy, Spectra-Phi, as well as data processing sessions on 4D-STEM and MicroED. Participants were guided through practical exercises using electron microscopes and image processing software. This hands-on experience was invaluable, allowing us to apply theoretical knowledge to real-world scenarios. The instructors were patient and skilled, providing personalized guidance to ensure that each participant could make the most of the practical sessions.

Meal/tea breaks

The school fostered a collaborative and engaging environment, facilitating interactions among participants, instructors and guest speakers. Networking sessions and group activities allowed attendees to exchange ideas, discuss challenges and explore potential collaborations. The diversity of backgrounds among participants enhanced the overall learning experience, providing a holistic perspective on the applications and challenges of electron crystallography in various scientific disciplines.

Poster sessions

The Electron Crystallography School also provided a platform for students and early-career researchers to showcase their research projects and findings. The poster sessions enabled attendees to gain deeper insights into the ongoing research in the field. This exposure to diverse projects and methodologies broadened our understanding of the potential applications of electron crystallography across different scientific domains.

Conclusions

The Electron Crystallography School was a comprehensive and well-organized program that delivered a profound learning experience. The combination of theoretical lectures, hands-on sessions, networking opportunities and exposure to cutting-edge research positioned participants to apply their new-found knowledge and skills in their respective fields. The school not only expanded our understanding of electron crystallography but also cultivated a sense of community among participants, fostering future collaborations and advancements in this dynamic field. I am confident that the knowledge gained at the Electron Crystallography School will significantly contribute to my research and academic endeavours.

Huyen Pham, Monash University, Australia

My name is Huyen Pham, a research fellow at the School of Physics and Astronomy, Monash University, Australia. I am extremely grateful and excited to have been part of the community attending the Electron Crystallography School, particularly after the hard period of COVID-19 lockdown and travel restriction. As a dedicated researcher in the field of materials characterisation by electron microscopy, I am always hungry to approach and acquire more knowledge in this topic. Participating in this event gave me an opportunity not only to expand my personal network but also to learn more fundamental knowledge and catch up with up-to-date progress in electron crystallography from famous scientists around the world. The school was well organized with a series of lectures on a wide range of topics including the fundamental theory of convergent-beam electron diffraction (CBED), 4D scanning transmission electron microscopy (4D-STEM) and 3D electron diffraction (3D-ED) together with historical background, software demonstrations and hands-on tutorials. This experience will truly support my growth and passion to be a researcher in electron microscopy. I also would like to thank the IUCr for committing to give me an IUCr grant, which strongly supports my travel costs and other necessary expenses.

Sepideh Rahimi, University of Antwerp, Belgium

I'm writing to convey my heartfelt appreciation for the Young and Early Career Scientist Award I had the privilege of receiving from the IUCr during the Electron Crystallography School at Monash University. This recognition has played a crucial role in facilitating my participation in this educational program. Your support means a lot to me, and I'm sincerely grateful for it. The experiences I gained have been immensely enriching and have contributed to my professional and personal growth.

The school allowed me to deepen my knowledge of 4D-STEM and CBED, gave me insights about developing my *in-situ* liquid experiments and provided valuable comments and ideas from famous experts in the field. I also had the opportunity to establish connections and collaborate with peers and mentors from around the world.

In terms of personal development, the experience broadened my horizons and enhanced my intercultural skills. It was an unforgettable experience that will undoubtedly benefit my future endeavors.

I am profoundly grateful for the support the Young and Early Career Scientist Award provided, which made this transformative journey possible. I am committed to utilizing the knowledge and experiences gained during this trip to further advance my research and contribute to the scientific community.

Once again, thank you for believing in my potential and supporting my academic and professional pursuits. I am truly honored to be a recipient of this prestigious award.

Please convey my gratitude to the members of the selection committee and all those who make these awards possible. I look forward to the opportunity to share the outcomes of this experience with you shortly.

Alaa Shaikhqasem, Martin-Luther Universität Halle-Wittenberg, Germany

I had the privilege to attend the Electron Crystallography School (ECS2023) which took place in August 2023 at the prestigious Monash University. My primary focus lies in 3D electron diffraction. The school presented a distinctive opportunity to connect with pioneering scientists who are actively shaping and sharing cutting-edge advancements in this field. Furthermore, this international event brought together participants from diverse backgrounds and experiences, creating a rich environment for exchanging ideas and establishing collaborations. The ECS2023 school provided me with an opportunity to present my work on 3D electron diffraction of protein crystals. Additionally, throughout the program, I acquired an extensive knowledge base in the field of electron diffraction, covering a wide range of topics including the following:

Advances in methods development and application

Sample preparation

3D electron diffraction data collection

Data processing for small molecules and macromolecules

Structure refinement and model validation.

How did the IUCr grant help?

Traveling from Germany posed financial challenges due to limited funds for travel, accommodation and expenses during my stay for the school. In this context, the IUCr grant proved to be a significant source of support, facilitating attendance and accommodation during the school.

I feel incredibly privileged to have been selected for the IUCr award, and I am grateful for the opportunity. I would like to express my heartfelt appreciation to Professor Laure Bourgeois and Dr Hongyi Xu for organizing the school and for their exceptional support and guidance throughout the duration of the event.

Yu Zhang, Monash University, Australia

As a student specialising in electron crystallography, receiving the IUCr Young and Early Career Scientist Award to attend the Electron Crystallography School 2023 has been a truly transformative experience. It provided me with a unique platform to engage with preeminent experts in the field, leading to enriching discussions and invaluable learning opportunities.

The sessions were nothing short of illuminating, particularly in revealing the remarkable capabilities of 4D-STEM and MicroED/3D-ED techniques. I was captivated by the hands-on laboratory demonstrations of 4D-STEM data collection led by Matthew Weyland, as well as the insightful discussions on post-processing of 4D-STEM by Jian-Min Zuo and Bryan Esser, each employing different software platforms, showcasing the diverse approaches to 4D-STEM data processing.

Moreover, the demonstrations by Colin Ophus, Scott Findlay and Hamish Brown, demonstrating the simulation of 4D-STEM using Python, were exceptionally intriguing. The talks covering precession electron diffraction and MicroED/3D-ED further deepened my understanding of these cutting-edge topics, highlighting the transformative potential of these techniques in structure determination, and significantly enhancing my insights. The subsequent industry speeches provided me with a profound understanding of the current priorities of leading companies, which has inspired my future learning and research. In summary, this masterclass has offered me a broader perspective on electron crystallography, allowing me to venture beyond the confines of my own research domain. I am sincerely grateful to IUCr for affording me this remarkable opportunity to participate in ECS2023.

Cheng Zhao, Monash University, Australia

The electron crystallography school (ECS) was truly an unforgettable experience. It was the first time that I had met with academics and researchers that I had repeatedly read about in the literature and textbooks.

ECS was well organised from the very beginning to the end. The program included a variety of areas in electron microscopy/electron diffraction. As an electron microscopy student, I was amazed and inspired by the continuous exploration people had put into developing techniques and even building up their own equipment for certain experiments. I was also very interested in all the demonstrations on newly developed simulation techniques. The ‘new for me’ information on three-dimensional electron diffraction was also a very interesting aspect that I had never thought to be so useful before.

Another point that made this school so different was that it started with very fundamental knowledge with few information barriers that I’m sure helped a lot of students who were not very familiar with electron crystallography.

Some of the most inspiring mentality that I learned was to always have faith in yourself (research-wise) and not be discouraged by other people’s words. On the other hand, one should have an open heart to the work of others and try your best to appreciate their work rather than doubting it.

This grant was of great help in covering my travel expenses. I am sincerely thankful to the selection committee.

Yi Zhou, ShanghaiTech University, China

This was my first time in attending such an overseas international conference. I had a fantastic experience at ECS2023, because of not only the thrilling lectures on both fundamental and cutting-edge science and technology about convergent-beam electron diffraction (CBED), four-dimensional scanning electron microscopy (4D-STEM) and three-dimensional electron diffraction (3D-ED) but also the chance to discuss face to face with pioneers and talented young scientists from all around the world in these fields.

During the school, I was very impressed by the quantitative analysis of CBED data by Professor Jian-Min Zuo from the University of Illinois at Urbana-Champaign (UIUC) and Professor Philip Nakashima from Monash Centre for Electron Microscopy (MCEM). The unit cell, symmetry, sample thickness, atom

positions and even orbitals can be analyzed. There were also a lot of lectures that showed us many useful software packages for processing 4D-STEM data with the speakers giving detailed instructions on how to use the software. Although I don’t work on this field, it still inspired me a lot. Lectures on 3D-ED and kinematical and dynamical structure refinement taught me a lot, which will benefit my experiments very much.

I was very honored to give a poster presentation on the evening of the first day of this electron crystallography school to present my up-to-date work about locating the guest species on metal–organic frameworks by 3D-ED. Several other talented young peers also presented their beautiful work, covering different materials and various techniques. It’s really good to know what others are doing and communicate with them.

Finally, I would like to say thanks to the organizers, Professor Laure Bourgeois and Hongyi Xu, for providing me with such a good platform to learn from others and promote myself. At the end of this school, I was awarded an “IUCr Young and Early Career Scientist Award”. This IUCr grant not only provided me with financial support but also gave me a lot of motivation. This is a kind of recognition for my previous research and encouragement for my future career.

MEETING REPORT

12th Belgian Crystallography Symposium



Luc Van Meervelt

More than 70 participants took part in the 12th Belgian Crystallography Symposium (BCS-12), which was held in the Academy Palace in Brussels on 18 October 2023. The National Committee for Crystallography organizes this symposium at biennial intervals to promote contacts between Belgian scientists using diffraction and microscopy techniques for studies in the fields of chemistry and physics, material sciences, earth sciences and life sciences. Because one of the main objectives is to give young researchers an opportunity to present their results, the symposium program includes, in addition to plenary lectures, flash and poster presentations and short lectures by PhD students and postdocs.

During the opening lecture by Professor Dorthe Ravnsbœk (Aarhus University, Denmark) a nice overview was given of how *operando* synchrotron X-ray diffraction and total scattering can be combined with pair distribution function (PDF) analysis to elucidate the structural evolution in a series of rechargeable battery electrode materials, which undergo varying degrees of disordering during charging or discharging. The morning session continued with nine flash presentations, including three from our sponsors.

Before lunch, a new microfluidics-based method for time-resolved cryo-EM sample preparation was presented by Professor Rouslan Efremov (Free University Brussels). The method was developed for the study of molecular machines, and its application to the GroEL/ES chaperonin system required for assisted folding of many proteins was demonstrated.

During the lunch break, participants had time to visit the poster session and our sponsors.



Romy Poppe (left) receives her IUCr Journals award from Professor Luc Van Meervelt.

In the afternoon Dr Matthew Lightfoot (Cambridge Crystallographic Data Centre, UK) highlighted the new possibilities with the Cambridge Structural Database, containing today more than 1.25 million structures, and its associated software. The knowledge derived from the structural data contained in the database has underpinned fundamental chemical discoveries and played a key role in designing new materials from drugs to pigments and beyond. The afternoon session ended with seven shorter lectures given by young researchers.

During the reception, two CCDC prizes were awarded to Marek Beliš (Ghent) and Thi Quintelier Matthias (Antwerp), together with the IUCr Journals prize for Romy Poppe (Antwerp).

This BCS-12 meeting was sponsored by Bruker AXS, UCB, Rigaku, CGB-CBB, CCDC and IUCr Journals.

MEETING REPORT

2023 Meeting of the Crystallographic Society of Japan



Kazuya Hasegawa, Hiroyoshi Matsumura

The 2023 Annual Meeting and General Assembly of the Crystallographic Society of Japan (CrSJ2023) was held at Yamaguchi University from 27 to 29 October 2023. In total, 273 crystallographers participated in the meeting, there were 160 oral and poster presentations covering all aspects of crystallography, three award lectures and five symposia. The Young Crystallographers Meeting 2023 was also held as one of the scientific sessions. Prior to the annual meeting, a satellite workshop on powder diffraction and total scattering was held on 26 October.

The annual meeting started with the general symposium 'Expanding Crystallography into Structural Science in Drug Discovery' (organizer: Professor K. Iwasaki, Tsukuba University). More than half of the total attendees of the meeting participated in this symposium despite the diversity in the attendees' professions. Four more symposia, also determined by open proposals, were held in parallel on day 3: 'Present Status and Future Prospects of Coherent X-Ray Diffraction Imaging' (organizer: Professor M. Nakasako, Keio University), 'Harmonic Interplay between Molecular Flexibilities and Crystal Rigidities' (organizer: Dr H. Sugiyama, CROSS), 'Protein Crystallographers Look at a New World Through Cryo-Electron Microscopy' (organizer: Dr N. Muraki, Keio University) and 'Crystallography on New Material Synthesis and Process Development Using High Pressure' (organizer: Professor T. Shimada, Hokkaido University).



The general symposium on the first day.

At the CrSJ Awards Ceremony, the Nishikawa Award was presented to Professor Tetsuya Ishikawa for his research 'A New Era in Crystallography Brought About by the Realization of Ultra-bright Synchrotron Radiation Facilities: SPring-8, SACLA and Beyond'; the Research Award was presented to Professor Masahiro Fujihashi (Osaka Medical and Pharmaceutical University) for his research 'Elucidation of Enzyme Mechanism as well as Exploration and Design of New Enzymes, Based on Crystal Structures'; and the Young Crystallographer Award was presented to Professor Yuki Takayama (Tohoku University) for his research 'Development and Application of Multishot Coherent X-ray Diffraction Imaging'.



The recipients of the 2023 CrSJ Awards with the President of CrSJ. Left to right: Professor A. Nakagawa (President), Professor T. Ishikawa, Professor M. Fujihasi and Professor Y. Takayama.

Five young scientists were honored with Student Presentation Awards based on their poster presentations on the first day: Mibuki Hayashi (University of Tsukuba) and Kazuki Hiraoka (Tohoku

University) in the physics and mineralogy field, Shun Sumikawa (University of Hyogo) in the chemistry field, and Keishiro Uda (Kyusyu University) and Midori Uenaka (Osaka University) in the biology field.



The five Poster Awardees at the banquet. Left to right: M. Hayashi, M. Uenaka, S. Sumikawa, K. Hiraoka and K. Uda.

The Young Crystallographers Committee organized a mini-symposium on the second day. Two invited young scientist speakers gave research presentations, and two graduate students presented their activities at IUCr2023. After the presentations, 66 participants, including young researchers and graduate students over several research fields, were separated into seven tables for group discussions. At each table, participants discussed and shared information on their research/campus life through crystallography.



Group photo at the Young Crystallographers mini-symposium.

A satellite workshop titled 'Fundamentals and Practices of New Analytical Methods in Powder Diffraction and Total Scattering' was held in collaboration with Rigaku Corporation and had 35 participants. The purpose of the workshop was to provide a program for researchers who are interested in new analytical

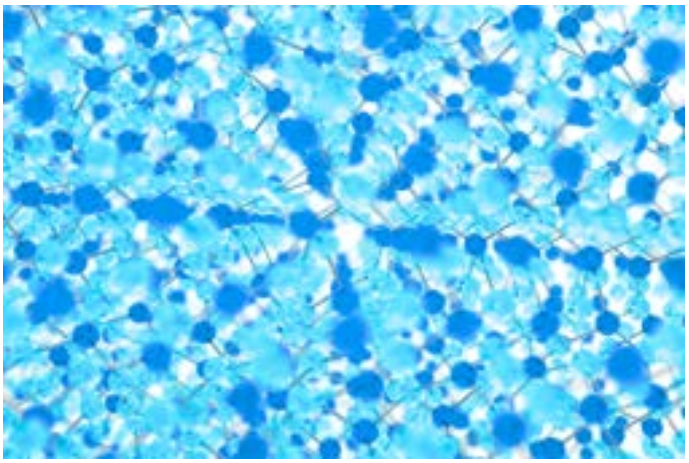
methods but are not confident in using them because they do not understand the fundamentals well or do not know how to apply them in practice because there are no experienced researchers in their institutions. Dr Hideo Toraya, the developer of the Direct Derivation (DD) method, an innovative quantitative analysis method using powder diffraction, gave a lecture on the basics of the DD method. Dr Masatsugu Yoshimoto presented the basics of the Pair Distribution Function (PDF) method and the Reverse Monte Carlo (RMC) method for total scattering pattern analysis. As a practical version of these analysis methods, Dr Miki Kasari demonstrated the analysis of demo data using Rigaku's *SmartLab Studio II* software.

The chair of the organization committee was Professor A. Nakatsuka (Yamaguchi University) and the program committee was chaired by Professor K. Komatsu (University of Tokyo).

The next annual meeting will be held on 8–10 October 2024 at Nagoya University, Aichi, Japan. The organization committee chair is Professor L. Chavas (Nagoya University) and the program committee is chaired by Professor S. Aoyagi (Nagoya City University).

NOTICE

CCDC news and updates



CSD Data Release (November 2023)

The fourth data release of 2023 adds 10,837 structures (11,411 new entries) to the Cambridge Structural Database (CSD). This takes the total size of the database to 1,254,560 structures (1,284,316 entries). This full release includes improvements to existing entries and new entries. In addition, knowledge bases like Mogul and IsoStar have been updated.

Find out more about our releases and this latest data update here.

November 2023 Update on Our Ongoing Investigations into Structures Associated with a Pre-print on a Papermill in Crystallography

In April 2023 we provided an update to confirm 209 of the implicated structures had been retracted from the CSD following the retraction of 125 associated publications. These retractions left 783 implicated structures under investigation.

Working closely with publishers and our community, we are following COPE guidelines as our investigations progress. We continue to add editorial comments to entries to highlight information that may be relevant so users can select fit for purpose data. Read more.

Recent Blogs

Investigating Solid Form Stability: Understanding Hydrogen Bond Propensity in *Mercury*

Mercury allows you to view, analyse and understand molecular structures and their properties. By exploring 3D structures, you can get a deeper understanding of the geometry of molecules, the way molecules pack together and what voids and channels exist within a structure.

This blog explores Hydrogen Bond Propensity, a component within CSD-Materials that studies the hydrogen bond network in a crystal structure, which was presented during the CCDC Virtual Workshop in October. Read the blog to learn more.

Unlocking Solid Form Innovation in CSD-Materials

CSD-Materials is a software suite that supports solid form development for crystal forms in the pharmaceutical and agrochemical industries. To enhance solid form reporting and research, the CSD Python API has been extended to cover more of the CSD-Materials suite, including parts of the Solvate Analyser, Hydrate Analyser and Aromatic Analyser components. Read the blog to learn more.

Improved CSD Torsion Data in *GOLD*

GOLD is the validated, configurable protein–ligand docking software for expert drug discovery, used for virtual screening through lead optimization. The torsion distributions sampled by *GOLD* during protein–ligand docking have been improved, including re-built and enhanced torsion distributions using the latest CSD and *Mogul* knowledge. Read the blog to learn more.

Upcoming Events

Visit our events page for more details on dates and topics. The next two webinars are as follows:

Accelerated, Accurate Drug Discovery using Enhanced Torsion Distributions, 25 January 2024

The Cambridge Structural Database in Electronics Research. Predicting Coercive Fields in Organic Proton-Transfer Ferroelectrics, 21 February 2024

If you would like to suggest topics for our workshops, webinars and CSDU online training modules in 2024, please email us at hello@ccdc.cam.ac.uk.

Free Online Courses

Learn more about the CSD, how to use CSD software and data to inform and advance your research, and how cheminformatics and structural chemistry can be applied to problems in the discovery and development of new molecules and materials.

The CSDU is a series of free on-demand training modules to learn at your convenience. Start anytime here.

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OBITUARY

Hendrik (Henk) Schenk (1939–2023)



Céleste A. Reiss

Henk Schenk passed away on Thursday 14 September 2023. He was a very amiable, good-natured crystallographer who contributed a great deal to the Dutch and international crystallographic communities.

Henk, born in Koog aan de Zaan, studied chemistry at the University of Amsterdam (UvA) and learned crystallography from Caroline MacGillavry, with whom he also obtained his PhD with the thesis *Automation of the symbolic addition method: Application to some compounds from the vitamin-A chemistry* in 1969. He developed the 'direct method' program *SIMPEL*, which used triple-product phase relationships for *ab initio* phasing; later the so-called 'quartets' and 'quintets' phase relationships were added. Henk worked and published with Herbert Hauptman (van der Putten *et al.*, 1980), who received the Nobel Prize in Chemistry in 1985 with Jerome Karle for 'their outstanding achievements in the development of direct methods for the determination of crystal structures'.

Henk became a personally appointed Professor of Direct Methods in Crystallography at UvA in 1980. Henk liked to teach, which resulted in a pamphlet for the Commission on Crystallographic Teaching of the International Union of Crystallography (IUCr) in 1984 (*An Introduction to Direct Methods*, https://www.iucr.org/education/pamphlets/17). In The Netherlands, he played a big role in the 'direct methods' discussion group that met regularly at the beginning of the 1980s.

In 1988, the position of Chair of Chemical Crystallography at UvA was established and assigned to Henk. He held this position until his retirement in 2004. Henk gathered a large group of students from The Netherlands and abroad who enjoyed the academic freedom given to them. Always searching for new scientific topics, Henk could explore a whole new area when his group obtained an X-ray powder diffractometer at the beginning of this century. Structure solution from X-ray powder data was still in its infancy and provided great opportunities for new developments, from software to exploring historical paints with X-rays. He was strongly involved in the Dutch–Belgian Beamline (DUBBLE) at the ESRF in Grenoble, which resulted in many publications and theses from his students. One of his most beloved subjects was the phase behavior of chocolate, perhaps because he lived remarkably close to a chocolate factory. In addition to his numerous scientific publications, Henk was also one of the Editors of *International Tables for Crystallography* Volume H: *Powder Diffraction* (published in 2019) and a Co-editor for *Acta Crystallographica Section A* from 2008 to 2021. He also wrote a survey of crystallography in *De geschiedenis van de scheikunde in Nederland* deel 3 (*The History of Chemistry in the Netherlands*, Part 3; Homburg & Palm, 2004).

Henk held many different board positions, including serving on the IUCr's Executive Committee from 1993 to 2005 and as IUCr President from 1999 to 2002. He was President of the Dutch Chemical Society

(KNCV) (in 1984) and the Dutch Fundamental Research Community for Crystal and Structural Research, as well as Dean of the Chemistry Faculty of the UvA (in 1994). On 30 March 1990, he founded, together with Roeli Olthof-Hazekamp, the Dutch Society for Crystallography, of which he was the first President and later became an honorary member.

Henk was a true citizen of the Zaanstreek, the industrial area north of Amsterdam: he was straightforward and loathed injustice. After Hugo Rietveld received all the credit for the ‘profile method’ for structure refinement from powder diffraction data, which became known as ‘the Rietveld method’, Henk and Bob van Laar published an article in *Acta Crystallographica Section A* (van Laar & Schenk, 2018) about its history. Based on this, Henk advocated referring to this method, first described by Loopstra & Rietveld (1969), as the ‘Loopstra method’ in recognition of the scientist who came up with the idea.

We lose with Henk a colorful and inspiring crystallographer, and we wish his family much strength with this loss.

References

Homburg, E. & Palm, L. (2004). Editors. *De geschiedenis van de scheikunde in Nederland*, Part 3. Delft University Press.

International Tables for Crystallography (2019). Volume H, *Powder diffraction*. Chichester: Wiley.

Laar, B. van & Schenk, H. (2018). *Acta Cryst*. A**74**, 88–92.

Loopstra, B. O. & Rietveld, H. M. (1969). *Acta Cryst*. B**25**, 787–791.

Putten, N. van der, Schenk, H. & Hauptman, H. (1980). *Acta Cryst*. A**36**, 897–903.

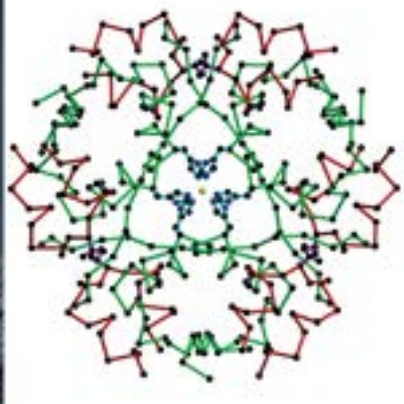
This obituary will also be published in *Acta Cryst.* (2024). A**80**.

For a list of papers by Professor Schenk appearing in IUCr journals click here.

OBITUARY

Robert H. Blessing (1941–2023)





Bob Blessing alongside a C^{α} trace of the T_6 bovine insulin hexamer [Smith, Pangborn & Blessing (2005). *Acta Cryst.* D**61**, 1476–1482].

Tim Bohen

Robert (Bob) Harry Blessing, a chemistry professor at the University at Buffalo (UB), NY, USA, and an emeritus senior research scientist at Hauptman-Woodward Medical Research Institute (HWI), died on 30 October 2023 at the age of 82. Considered a leader in the field of high-resolution experimental crystallography for electron density modeling, he collaborated on numerous research papers and spoke at many national and international conferences.

Born in Wilkes-Barre, PA, he graduated in 1962 from King's College in Wilkes-Barre. After completing a PhD in inorganic and physical chemistry at Ohio University in 1970, he held postdoctoral positions at the University of Lund, Sweden; the University of Pittsburgh; and UB. After four years as an Assistant Professor of Chemistry at Mercyhurst College in Erie, PA, he moved to Buffalo in 1978 to become a Research Scientist at HWI, formerly the Medical Foundation of Buffalo. There, he worked with emeritus researcher Dr G. David Smith on the crystal structure of insulin. He also developed algorithms and software for crystallographic data reduction and error analysis that are widely used in laboratories worldwide. He co-authored publications with Smith and 1985 Nobel Prize in Chemistry winner Herbert Hauptman.



In good voice. From left to right, Wilson Greatbatch, Herbert Hauptman, Bob Blessing and Lodovico Riva di Sanseverino sing at the 75th birthday celebration for Nobel laureates Herbert Hauptman and Jerome Karle in Buffalo in 1992. Photo contributed to the IUCr gallery by W. L. Duax.

Dr Blessing continued his work at HWI after he was appointed an Associate Professor of Chemistry at UB in 1991. He was promoted to Full Professor in 2001, and during that same year helped design the graduate studies program for the Department of Structural Biology in UB's Jacobs School of Medicine and Biomedical Sciences. He later served as the Department's Director of Graduate Studies and Chair.

On four occasions, he was a visiting professor in the crystallography laboratory at the Université Henri Poincaré, now Université de Lorraine, in Nancy, France, where he had a long collaboration with Claude Lecomte, Professor of Crystallography and Physics.

He was President of the Pittsburgh Diffraction Society and an active member of the American Crystallographic Association.



From left to right, Akihito Yamono, Tony Linden, Bob Blessing, Ludger Häming, Ton Spek, David Watkin and Larry Falvello, speakers at the Microsymposium on Absorption Corrections at the 18th IUCr Congress in Glasgow, UK, in 1999.

Dr Blessing is survived by his wife of 61 years, Barbara Ann; a daughter, Kimberly Blessing, a philosophy professor at Buffalo State University, and son-in-law, Tim Bohen; and two grandsons. Another daughter, Kirsten Blessing-Hanagan, a nurse in the neo-natal intensive care unit at the former Women and Children's Hospital, died in 2006.

For a list of papers by Dr Blessing appearing in IUCr journals click here.

PRESS RELEASE

Anton Paar looks forward to its 60th anniversary celebrations



Barbara Puhr

Pioneer in non-ambient X-ray diffraction

When we at Anton Paar introduced the HTK 10 high-temperature chamber back in 1964, we made our mark in the history of non-ambient X-ray diffraction. The HTK 10 high-temperature chamber was capable of heating samples up to 1600 °C in order to study their structural changes by X-ray diffraction during heating.

Prior to this, non-ambient X-ray diffraction of various materials was mainly done with home-made equipment, but there was no real commercial heating chamber available on the market. This changed when we entered into this market 60 years ago. Since then, our knowledge and experience in X-ray diffraction, especially under non-ambient conditions, has steadily grown. This has led to our current broad portfolio of non-ambient X-ray diffraction attachments for studies between –190 °C and +2300 °C under different atmospheres (dry and humid) and pressures, as well as mechanical or electrical loads. Along with this complete portfolio, we also create customized solutions for our customers, something that helps make Anton Paar the market leader in non-ambient XRD.

60th anniversary celebration

In 2024, we will proudly celebrate our first milestone in the field of X-ray diffraction. As part of the anniversary celebrations, we're organizing the **XRD excites: Non-Ambient XRD & Beyond Symposium**, a scientific meeting with a strong focus on non-ambient X-ray diffraction in Graz, Austria, from 9 to 11 July 2024. In addition, our Anton Paar subsidiaries will be organizing regional non-ambient X-ray diffraction workshops. Throughout the anniversary year, we have lots of things planned.

For more information, follow us on LinkedIn or click here.



Contact: barbara.puhr@anton-paar.com.

IUCR SUPPORTED EVENTS

IUCr supported meetings

These forthcoming meetings are supported by grants from the IUCr Calendar Committee.



11th Oct 2026 - 16th Oct 2026

Indaba10

Skukuza, Kruger National Park, South Africa



5th Dec 2026 - 10th Dec 2026

African Materials Research Society (AMRS 2026)

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

This is a list of meetings of interest to crystallographers occurring within the next twelve months, as recorded in the IUCr Calendar of Events. Please let us know of any that are missing by completing this form or sending an email to forthcoming.meetings@iucr.org.



Indaba10 South Africa 11th Oct 2026 - 16th Oct 2026



Synchrotron Radiation: Science, Knowledge, Innovations, Future (SKIF-2026) Russian Federation 18th Oct 2026 - 23rd Oct 2026



CCP-EM/Diamond Icknield Workshop United Kingdom 9th Nov 2026 - 13th Nov 2026



Instruct-ERIC hands-on workshop on Advanced cryo-FIB-SEM methods Germany 9th Nov 2026 - 13th Nov 2026



Crystal36-AXAA 2026 Meeting Australia 26th Nov 2026 - 2nd Dec 2026

African Materials Research Society (AMRS 2026) Kenya 5th Dec 2026 - 10th Dec 2026

Joint Polish-German Crystallographic Meeting 2027 Germany 15th Feb 2027 - 18th Feb 2027