INTERNATIONAL UNION OF CRYSTALLOGRAPHY

# IUCr Newsletter

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LETTER FROM THE PRESIDENT

# Now is the time!




From left to right: David Rose, ACA Immediate Past President; Hanna Dabkowska, IUCr President; and Bill Duax, former IUCr President/*Newsletter* Editor, at the IUCr booth during ACA2022.

Hanna Dąbkowska

In the last six months I have done a lot of things we were not encouraged to do at the height of pandemic.

I was able to attend IN PERSON two IUCr Finance Committee meetings and one IUCr Executive Committee meeting as well as two — very well organized — Regional Associate meetings, both in amazingly beautiful locations: ACA2022 in Portland, OR, USA (hybrid meeting, 480 in-person and 83 online participants, organized by Brandon Mercado, S. Powell, Anna Gardberg and Carla Slebodnick) and ECM33 in Versailles, France (about 900 participants, chaired by Sylvain Ravy, Andy Thompson and Jean-Paul Itié).





Left: An ACA Fellows meeting in Portland in 2022. Right: Manfred Weiss, IUCr Executive Committee member; Marvin Hackert, former IUCr President; Gerald Audette, ACA Canadian Representative; Amy Sarjeant, *Acta Cryst. C* Co-editor; and Hanna Dabkowska, IUCr President, at the IUCr booth during ACA2022.

I took part in the 7th European Conference on Crystal Growth (ECCG7), professionally organized by Matias Velazquez in Paris, France.





Left: ECCG7 Chair Matias Velazquez and Hanna Dabkowska during the gala dinner cruise on the Seine. Right: A meeting of the IUCr Commission on Crystal Growth and Characterization of Materials in Paris in July 2022.

I also participated in the recent IUCr Journals Management Board meeting (by Zoom). I was impressed by the huge amount of innovative work being done for the IUCr Journals under the leadership of Andrew Allen and Peter Strickland.

I met a lot of cool people with crystallography at heart: researchers, students, young scientists, volunteers, our staff — I mean I met many of you.

And — as usual — I am full of admiration for the great science you are all doing and for the innovative ways you are sharing your knowledge. Sharing with your peers, students and colleagues — on site and in other countries. I feel a lot of enthusiasm; I hope it will translate into many successful publications — contributing to many successful careers — not only in crystallography but also in the very diversified area of structural sciences.

We are just coming out of the pandemic and are still in the shadow of the devastating war in Ukraina but please realize the following:

Now is the time to **strengthen** collaboration among different countries and institutions.

Now is the time to **enlighten** many of our colleagues (proud physicists, chemists, biochemists and engineers) that their research is based on an appropriate understanding of (crystallographic) structure of any material they are working on.

Now is the time to **organize** a School or a Workshop. The Executive Committee of the IUCr has decided to rename the Calendar Committee (the proper name was Sub-committee on the Union Calendar) to **Meeting Support Committee** (MSC). I assume that this is a good decision as the new name better reflects what we are doing. Here I would like to thank Graciela Díaz de Delgado and the whole Calendar Committee team for the work well done in a very difficult time. At the same time I welcome Manfred Weiss as the new MSC Chair.

Now is the time to persuade your student to **sign up** for an (IUCr-supported) specific School or Workshop and to **enrol** in the *World Directory of Crystallographers*.

Now is the time to **register** for the Melbourne Congress, plan your contribution, check the program and decide how you want to participate.

Now is the time to **spread** our wings and encourage African researchers to continue developing research of their own. I admire the tireless work that Claude Lecomte, Michele Zema, Susan Bourne, JuanMa García-Ruiz, Yuki Kimura, Dave Billing and many others are doing in Africa. The African Crystallographic Association (AfCA), under the leadership of Delia Haynes, is expected to join the IUCr as a Regional Associate as soon as in Melbourne.

Now is also the time to **engage** with a science teacher in your local high school to take part in a local crystal growth competition (see here for an example recently reported in the *IUCr Newsletter*) — or any other of your favourite scientific activities.

I sincerely hope that you nominated a colleague or student for one of the IUCr Prizes (as when this *Newsletter* is published the deadline will have already passed). You can still make up your mind and think about a worthy candidate for the future.

We are the IUCr. We create and nourish global partnerships for developing structural science. We invent tools that other scientists are using. Our Journals and *International Tables* provide unparalleled expertise for a diverse approach to structural science. Our colleagues and partners build sophisticated equipment that — with a push of a button — solves difficult structures. And — with our Schools and Workshops — we create a community that understands that plenty of creativity and knowledge is needed to connect this "difficult to solve structure" with a real-world challenge: a new virus, a potential new drug, an efficient battery material or a low-cost, easily disposable food container.

And now is our time to do it all.

EDITORIAL

# Editorial

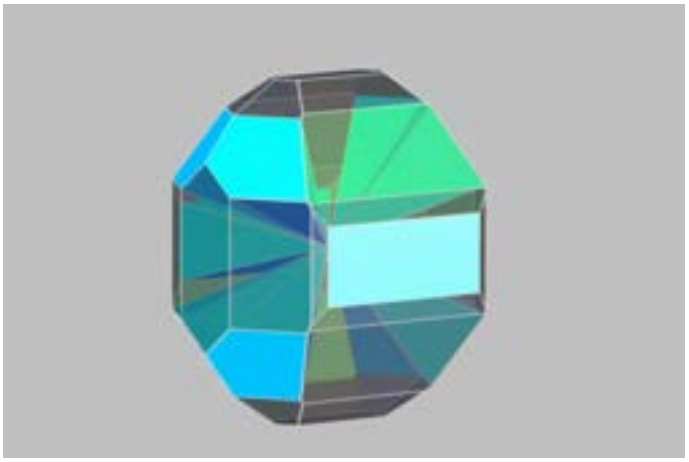


Image made by *WinXMorph* by Werner Kaminsky.

Mike Glazer

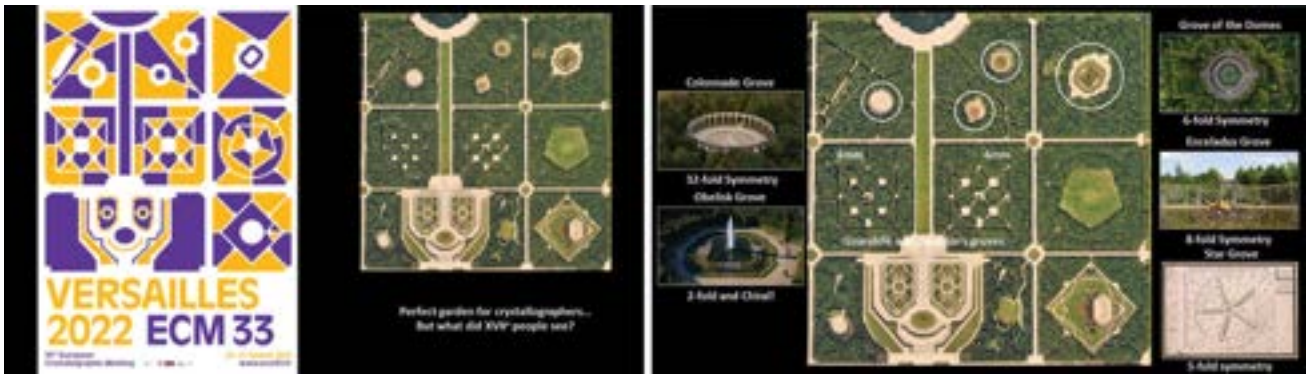
This summer has been sweltering here in the UK, sometimes making it difficult to concentrate on work. Climate change? Probably, and this holds a warning to us all for the future. So what do we have in this issue of the *IUCr Newsletter*?

Now, as scientists, we expect to announce our discoveries to the rest of the world through publishing in legitimate science journals. We normally expect that papers that appear in journals and have been properly refereed can be trusted to be written in good faith so they can be treated as reliable. That, however, is an ideal, which sometimes is open to deception, and untrustworthy publications do appear from time to time that pollute the scientific literature. This is despite the fact that reputable journals, such as our IUCr journals, go to enormous efforts to maintain standards.

In recent years, there has been a growth in suspect articles being published. Sometimes this is simply a matter of incompetence of the authors, and referees have not spotted the errors. Referees are only human, aren't they? But sometimes, there is a more malign reason. The pressures to publish as many papers as possible to gain job promotion or personal recognition are largely responsible for this. In April of this year, a paper appeared in which evidence of the existence was provided of a so-called "paper mill", designed to create hundreds of fake manuscripts. You can read the original report here. Such material is challenging to track down especially as the articles often appear in many different journals. The publication of such dubious material has even affected the Cambridge Structural Database, where 992 recent crystal structure papers have been found across several journals, raising suspicions of "paper mill" activity. Fortunately, the CSD has excellent ways to detect them for the most part, but of course, one can never be certain that some may have crept through. I also recall that Armel Le Bail has been particularly active in finding many suspicious examples (see, for example, his "crystallographic horrors" at http://cristal.org/CHM/CHM.html). It is worrying to see publications like this polluting the scientific literature. I, too, have seen, while refereeing, some examples of identical powder diffraction patterns that have been repeated elsewhere, even though the authors claim to be studying different materials. This is something that journal referees need to be aware of these days. A recent research report on paper mills from the Committee on Publication Ethics (COPE) & STM gives an idea of the wider problem.

On a lighter note, it is great to see the steady development of crystallography growing within the African continent. Owing to the work of crystallographers such as Claude Lecomte and the IUCr, it has been possible to establish a Senegalese Crystallography Association. This can only bode well for the development of our science in Africa. I am proud of the role played in this by the IUCr.

The meetings of the IUCr Regional Associates are always a highlight of the crystallographer's year, and in 2022 we are delighted to congratulate the European Crystallographic Association on the occasion of their 25th anniversary. For those of you wondering how come we've already reached the 33rd European Crystallographic Meeting (ECM33), it's because the ECA succeeded the European Crystallographic Committee (ECC), which was founded 50 years ago at the very first ECM. Read more in ECA Vice-President Arie van der Lee's article here. During the ECM33 Opening Ceremony, Co-Chair Sylvain Ravy related how the ECM33 logo was inspired by the gardens at the 17th century Château de Versailles, close to the meeting venue, and went on to describe the types of symmetry exhibited by some of the gardens' features (see slides below). The ECA's prestigious Perutz Prize went to Bill Clegg from Newcastle University (UK), a well-deserved winner for his contributions to crystal structure solution.




Opening Ceremony slides, courtesy of Sylvain Ravy. Logo design by Léo Ravy.

The 72nd ACA Annual Meeting also returned to an in-person gathering in 2022 and hosted sessions – some hybrid – in an expanded range of disciplines. Read a report here. The IUCr awarded poster prizes at both ACA2022 and ECM33; many congratulations to the winners (shown below)!




IUCr Journals Poster Prize winners. Left: Anna Jewczynko (University of Waterloo, ON, Canada) beside her winning poster at ACA2022. Right: Corentin Chatelier (CEA Grenoble and ESRF, France), Abigail Sudol (University of Southampton, UK) and Szymon Sobczak (Adam Mickiewicz University, Poznan, Poland) receiving their prizes from IUCr Vice-President Santiago Garcia-Granda at ECM33 (photo credit Laura Martin).

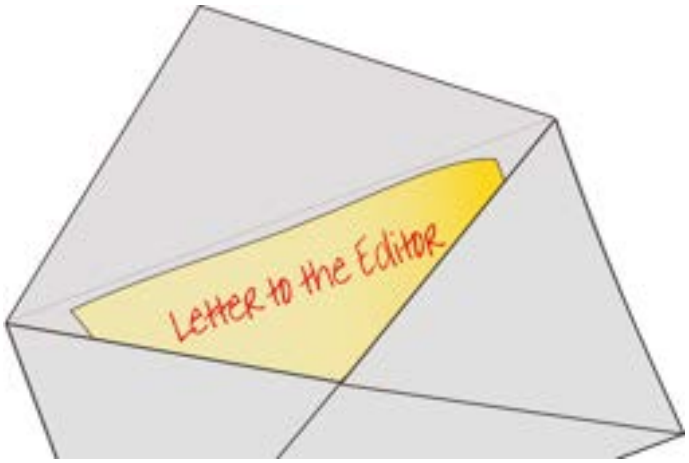
We look forward to the 17th Conference of the Asian Crystallographic Association, taking place in Jeju, Republic of Korea, from 30 October to 2 November 2022, and the 5th Meeting of the Latin American Crystallographic Association, which will be hosted by San José in Costa Rica from 28 to 30 November 2022.

Once again, the Hargittais have written an interesting article for the *Newsletter*, this time on the life of Don Caspar regarding his collaboration with the Nobelist Aaron Klug in connection with geodesic domes towards understanding virus structures. I always enjoy reading their contributions to the *Newsletter*.

Finally, in the previous issue of the *Newsletter*, Maureen Julian wrote about her experiences in Kathleen Lonsdale's laboratory in the 1960s. She asks if anyone else can recall those times to contact her at erie@vt.edu.

LETTER TO THE EDITOR

# Letter to the Editor




Eric Mittemeijer

I read, with interest, (i) your feature article "*The mystery of the Lady of the Lamp*" in *IUCr Newsletter*, Vol. 30, No. 1, and (ii) your editorial and (iii) the letter to the Editor by Stefan Dietrich, both in *IUCr Newsletter*, Vol. 30, No. 2. The scientist (crystallographer) Victor Mordechai Goldschmidt is nowadays mostly forgotten, yet, as a matter of fact, he is one of the founders of crystallography, with Federov and Groth, before the discovery of X-ray diffraction revolutionized the field.

I felt obliged to include in the second edition (2021) of my book "*Fundamentals of Materials Science*" (see https://link.springer.com/book/10.1007/978-3-030-60056-3) a short *Intermezzo* devoted to his achievements [see ch. 4 (*Crystallography*), pp. 120–121]. The two-circle goniometer named after Goldschmidt, of unsurpassed precision, found worldwide application. It is also worthwhile to remark that the highly skilled technician in Goldschmidt's group, Peter Stoe, later became the founder of a firm named after him, "Stoe", that still exists and produces X-ray diffractometers.

I have to admit that the above important facts were unclear to me during the longest part of my career. I knew, of course, the name Goldschmidt, but only with respect to his well-known table of atomic radii and the tolerance factor. I have now been living for a few years in Heidelberg. By chance, during a stroll across the "mountain cemetery" ("Bergfriedhof") of Heidelberg, I was suddenly, unexpectedly confronted with the grave of the scientist Victor Mordechai Goldschmidt (1853–1933). I thought I was standing before the grave of the man of the "Goldschmidt atomic radii" and the related "Goldschmidt tolerance factor". However, this interpretation was found to be utterly wrong!

The "Goldschmidt atomic radii" and the related "Goldschmidt tolerance factor" are due to the, indeed also famous, geochemist Victor Moritz Goldschmidt (1888–1947) (Victor **Moritz** Goldschmidt was related to Victor **Mordechai** Goldschmidt, via the mother of the father of Victor Moritz; I don't know if both Victors ever met).

Evidently, many have mixed up the two Victor Goldschmidts, who moreover have identical initials (V. M.). It has happened to me for many years, and it has also happened now to you (see Note [1] in your feature article). To put the record straight, it may be worthwhile to make the readers of the *IUCr Newsletter* aware of the distinction in achievements of these two great scientists.

As a final sad note, I may add that both Victors (Victor Mordechai Goldschmidt and Victor Moritz Goldschmidt), as Jews, suffered from Nazism, were subjected to severe harassment, had to leave Germany, and died before and after the Second World War, respectively.

FEATURE ARTICLE

# MAX IV Laboratory – a fourth-generation light source




Early morning at MAX IV, located in Lund, Sweden. Neighbouring neutron facility European Spallation Source, ESS, is visible in the upper right corner.

Emelie Hilner, with contributions from Aymeric Robert

MAX IV Laboratory is a Swedish national synchrotron laboratory that has been operating as a user facility since 2016. It is the successor to MAX-lab, which was in operation between 1987 and 2015. It offers access to 16 beamlines that provide modern X-ray spectroscopy, scattering/diffraction and imaging techniques to contribute to solving scientific questions. The latest additions to our beamline portfolio are ForMAX and MicroMAX.

MAX IV welcomes about 1000 users from academia and industry every year, which is expected to double in the coming years. About 75% of our users are affiliated with institutions from Nordic countries (Sweden, Denmark, Norway, Finland, Iceland). Our beamlines are open to academia, research institutes, industry and government agencies worldwide. Access is without charge for users who intend to publish their results in the open literature. It is granted based on the scientific merit and technical feasibility of science proposals submitted twice a year. Industry can also get access through a proprietary access program.

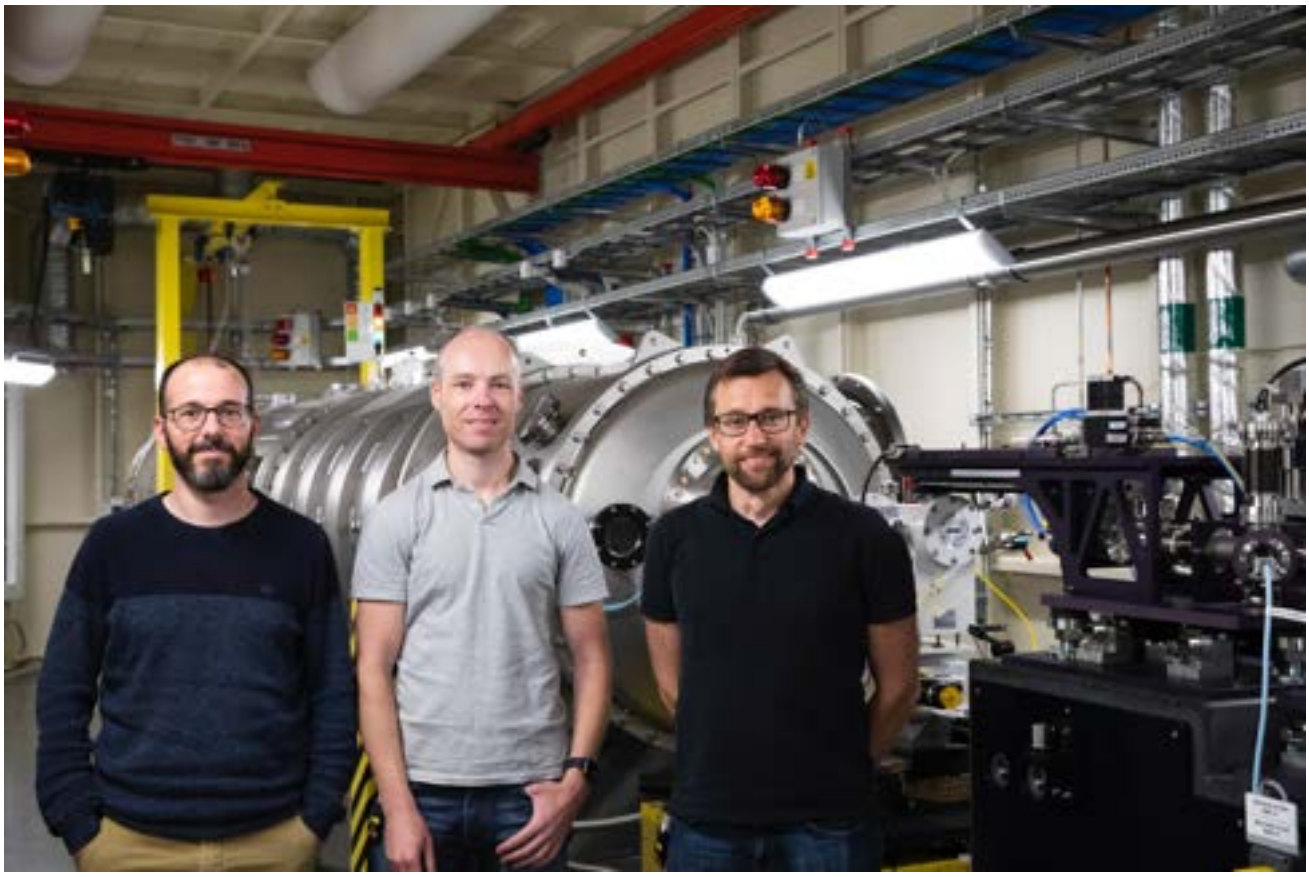
MAX IV is currently formulating a strategy for the upcoming years towards 2035 in collaboration with the user community. Our strategy will identify opportunities to address important scientific questions of high relevance to society that will translate into the definition of a set of new beamlines to continue to develop our beamline portfolio.

## The recently opened ForMAX beamline focuses on renewable materials

One of the newest additions to MAX IV is the ForMAX beamline that recently opened for users. A large part of the research at ForMAX will focus on developing materials and chemicals from renewable supplies and forest-based sources. ForMAX is financed by industry, universities and foundation partners in the Treesearch consortium.

An important focus area of ForMAX is characterising complex materials across a broad range of length scales. For example, the mechanical properties of wood originate from various hierarchical structures and sub-structures spanning from hundreds of micrometres down to the nanometre scales. This will be performed by combining full-field tomography with small- and wide-angle scattering. The experiment setup is built around a single sample table to allow switching between modes of operation without

moving the sample. Thanks to the large X-ray brilliance from our 3 GeV storage ring, ForMAX will extend conventional studies to the time-resolved realm, thus allowing *in situ* material processing to be followed.



The ForMAX beamline team, J. González, S. McDonald and K. Nygård (missing V. Haghighat), in the experiment hutch.

## Focus on dynamics and *in situ* studies

The superior performance of X-rays from small-emittance storage rings, such as those generated from our 3 GeV accelerator, create opportunities to develop analytical X-ray tools that rely on highly brilliant and coherent X-rays.

These can translate into providing experimental capabilities to tackle many scientific questions ranging from life sciences to nanoelectronics:

(i) For example, protein crystallography can benefit from intense X-ray beams with very small beam sizes at our BioMAX [1] and MicroMAX beamlines, thus providing more measurement opportunities with protein crystals of a small size. Previously challenging membrane proteins are essential for understanding illnesses such as Parkinson's and Alzheimer's disease.

(ii) A larger X-ray brightness opens unprecedented opportunities to perform time-resolved *in situ* studies. An excellent example is ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) at the HIPPIE beamline [2], where the spectroscopic details of gas molecules reacting on a catalytic surface can be followed under high-pressure conditions. As surface dynamics often change with pressure, it is critical to have access to realistic experimental conditions. A development with Oslo University's users is a novel hardware/software interface for time-resolved AP-XPS experiments. The combination of methods offers complementary spectroscopic and kinetic data about complex reaction mechanisms at surfaces.

(iii) A recent example is an experiment on the deformation dynamics of steel at the DanMAX beamline, which is of great importance for the steel beams used in a car to protect passengers in case of an accident. The speed of loading rate of the steel has an important impact on the resulting mechanical transformations that occur and has not been studied in this realistic way before. The very intense hard X-ray beam penetrates through the sample collecting data from its atomic scale structure while a loading

rig simultaneously pulls it.

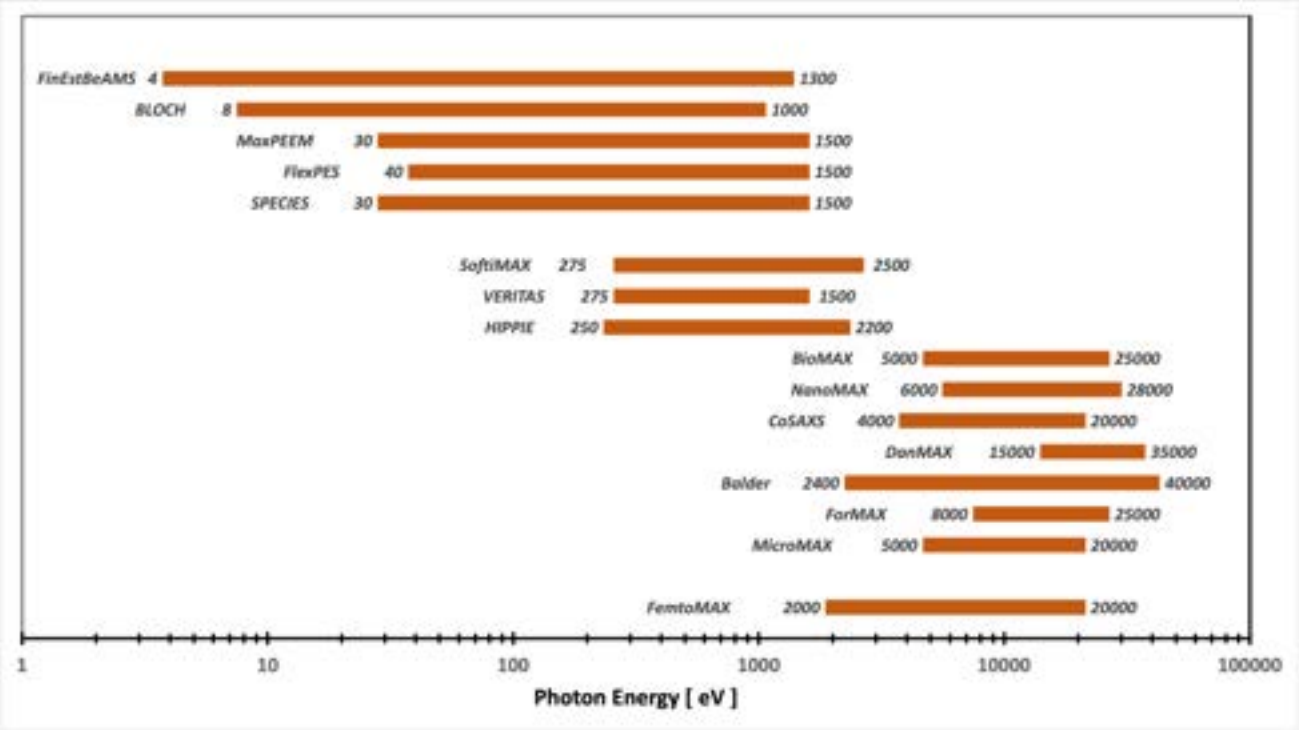
(iv) Nanoelectronics and energy materials are other areas that can tremendously benefit from focusing incident X-ray probes to small, micrometre and submicrometre sizes. A recent study using our NanoMAX beamline [3] addresses ferroelastic domains of metal halide perovskites, a promising material for future solar cells and light-emitting diodes.

(v) Small-emittance storage rings offer unprecedented opportunities to continue developing tools that exploit the large degree of X-ray coherence of these highly brilliant beams. This is, for example, the case with X-ray photon correlation spectroscopy (XPCS), which is being implemented at our CoSAXS beamline [4] and can uniquely probe the structural equilibrium and out-of-equilibrium dynamics of disordered amorphous matter, such as that found in soft-matter systems.

More examples can be found in the last edition of our annual science *Highlights*.

## An advanced accelerator complex with a 3 GeV MultiBend Achromat lattice storage ring

The MAX IV linear particle accelerator (linac) injects full energy into two storage rings of 1.5 and 3 GeV. They are reliable sources of X-rays with remarkable uptime of about 97% and each delivering more than 4000 beamline hours per year. This unique accelerator complex covers the production of X-ray photons over a broad energy range from vacuum ultraviolet (VUV) to hard X-ray (4 eV to over 40 keV) with no gaps in the photon energy spectrum. It is also possible to compress the electron bunches and feed a set of undulators at its end, producing X-ray pulses as short as 100 fs with a 10 Hz repetition rate to the FemtoMAX beamline [5]. The linac can also be used to seed a future soft X-ray free-electron laser.




Photon energy ranges for the 16 beamlines at MAX IV. The beamlines cover an energy range of 4 to 40,000 eV with no gaps.

The 528-metre circumference lattice of our 3 GeV ring has 20 bending sections or achromats, each including seven bending magnets in a MultiBend Achromat (MBA) structure instead of the two that were the standard until now for synchrotron sources of preceding generations. Based on this design, our 3 GeV ring was the first worldwide realization of a fourth-generation light source. Its small emittance laid the foundation for continuing developing tools that rely on X-ray beams with high brightness and a large degree of coherence.

The implementation of this novel lattice design posed several challenges that had to be solved, such as compact groups of magnets being machined into a common iron block and the space between magnet poles only allowing for a very narrow vacuum chamber between them. As an additional example, the inside of the entire vacuum chamber of our 3 GeV ring is covered in a non-evaporable getter coating to reach the necessary ultra-high vacuum conditions (https://cerncourier.com/a/max-iv-partnership-is-the-key/).

Most light sources around the world are either operating [ESRF (France), Sirius (Brazil)] or planning [Soleil (France), SLS (Switzerland), Diamond (UK), ALBA (Spain), APS & ALS (USA), SPring8 & NanoTerasu (Japan)] to use a hybrid-MBA design as inspiration. An exciting future of discoveries with these bright and coherent X-ray beams from fourth-generation light sources is ahead.

Contact for more information:

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IUCR ACTIVITIES

# Message from the IUCr Chief Executive Officer



The IUCr Executive Committee during their meeting in Versailles, France, in August 2022. Left to right: Sven Lidin (Immediate Past President), Jenny Martin, Bo Brummerstedt Iversen (General Secretary and Treasurer), Angela Altomare, Thomas Proffen, Hanna Dabkowska (President), Manfred Weiss, Graciela Diaz de Delgado and Santiago Garcia-Granda (Vice-President). Masaki Takata joined the meeting via Zoom.

Alex Stanley



My summer has been spent studiously, learning how to steer the ship of the IUCr, which has been magnificently helmed by Alex Ashcroft for the last five years. Many of the financial operations of the organisation were overhauled during Alex's tenure making my handover considerably easier than it was during his first weeks and I would like to extend my gratitude to him for answering my endless queries and questions. I wish him a very happy and productive retirement.

Towards the end of August, the Finance and Executive Committees of the IUCr met together in Versailles and it was a great opportunity to meet the elected members. During a special dinner, Hanna Dabkowska, on behalf of the Executive Committee, formally thanked Malcolm Cooper (Financial Convenor) for 25 years of guidance to the Finance Committee and Luc Van Meervelt for ten years' service as General Secretary and Treasurer, and congratulated Alex Ashcroft (Executive Secretary) on his retirement. Between meetings, I squeezed in a visit to ECM33 and caught the opening ceremony and exhibition – the start of what was a very successful and well-attended event. Many congratulations to the ECM Program Committee, AFC and all the members of the Local Organizing Committee.



From left, Malcolm Cooper, Luc Van Meervelt and Alex Ashcroft receive mementoes of their years of service to the IUCr from IUCr President Hanna Dabkowska, and Zoran Štefanić and Aleks Višnjevac chat to IUCr staff members Andrea Sharpe, Alex Ashcroft and Michele Zema at the IUCr exhibition stand at ECM33.

Why did I decide to join the IUCr office in Chester? Not only is it a welcoming and long-established community but the discipline of crystallography overlaps with such a broad range of scientific research. I would like to continue to build up connections with other communities to expand the horizons of the organisation particularly in the IUCr Journals. To do this, we must first identify the IUCr's purpose and goals. One way to do this is to define our 'Mission, Vision and Values' (MVV) as an organisation that will serve to provide us with a clear direction. You can imagine my delight when Jenny Martin (Executive Committee member) proposed during the Executive Committee meeting to undertake this exact MVV project. It was as if she had read my mind and you can expect to hear more on this later in the year.

As the Chester office embraces a dynamic and hybrid Work From Home arrangement, one of my first tasks is to begin the closure of No. 2 Abbey Square as the space is now surplus to requirements. In fact, it has become more of a storage unit for vast quantities of IUCr paperwork, rather than a functional office. A large part of this move will involve digitisation of historic documents that will eventually serve as an accessible archive for all. The recently refurbished Nos. 5 and 6 Abbey Square, where much of the editorial team are located, will remain and is the main contact address for the IUCr office.

IUCR ACTIVITIES

# IUCr meeting support




Participants at ICCOSS XXV, one of the many meetings supported by the IUCr.

Manfred S. Weiss



Manfred Weiss.

At the IUCr Executive Committee meeting held during ECM33 in Versailles, France, a decision was taken to rename the *Sub-committee on the Union Calendar* to the *Meeting Support Committee*. Dr Manfred Weiss was appointed as Chair of the Committee, succeeding Professor Graciela Delgado. Manfred is a macromolecular crystallographer and works at the BESSY II synchrotron of the Helmholtz-Zentrum Berlin,

Germany. He has served on the IUCr Commission on Biological Macromolecules and the Teaching Commission for many years, and has been co-editor of *Acta Cryst. D* and *Acta Cryst. F* and Section Editor of *Acta Cryst. F* from 2008 to 2017.

All requests to the Meeting Support Committee for the financial support of meetings, workshops, schools *etc*. should be sent to Manfred directly from now on at manfred.weiss@helmholtz-berlin.de.

IUCR CONGRESS

# Strong plenary speaker triumvirate confirmed for IUCr 2023




IUCr 2023 plenary speakers (from left): Professor Hideo Hosono, Dr Junko Yano and Professor Mark Spackman.

We are thrilled to announce that three world-leading experts in their field will headline IUCr 2023 in Melbourne: Professor Hideo Hosono from the Tokyo Institute of Technology, Japan; Dr Junko Yano from Lawrence Berkeley National Laboratory, CA, USA; and Professor Mark Spackman from the University of Western Australia, Perth, Australia.

## Hideo Hosono

Professor Hosono is renowned for his work on the creation of novel functional materials. Some of Hideo's noteworthy achievements include the design of transparent oxide semiconductors such as indium gallium zinc oxide (IGZO) and their thin-film-transistor (TFT) applications for state-of-the-art displays (OLED TVs are driven by IGZO-TFTs), creation of room-temperature stable electrides and their application to catalysts for ammonia synthesis, and discovery of high-$T_c$ iron-based superconductors. Hideo is an honorary and professor of Tokyo Institute of Technology and a group leader and distinguished fellow at the International Center for Materials Nanoarchitectonics (MANA) of the National Institute for Materials Science. He received a PhD in Applied Chemistry from Tokyo Metropolitan University in 1982, and became a professor of Tokyo Institute of Technology in 1999 via the Nagoya Institute of Technology and Institute for Molecular Science at Okazaki. He is a recipient of various honors including the Japan Prize, von Hippel Prize (MRS), J. McGroddy Prize (APS), Jan Raychman Prize (SID), Imperial Prize of the Japan Academy, Thomson Reuter Citation Laureate and a foreign fellow of the Royal Society.

## Junko Yano

Dr Yano's research has focused on problems of importance to energy, especially renewable energy sources. Her group uses X-ray spectroscopy and crystallography to understand biological and inorganic systems. For example, her lab has explored how in photosynthesis, plants use light to split water using a catalytic $Mn_4Ca$ cluster, and converting light energy into chemical energy. Since the advent of X-ray free-electron lasers (XFELs), her group has been using these facilities to study the catalytic systems, under functional conditions at room temperature. These methods allow one to study structure–function relationships by following the reactions in real time and the effect of the environment of the protein on the active site. Junko is a member of the Liquid Sunlight Alliance (LiSA), where she studies artificial photosynthetic systems, combining her interests in natural photosynthesis/metalloenzymes with inorganic systems that can be used to engineer practical devices. Since 2015, Junko has held the position of Senior Scientist, and Division Deputy for Science (since 2020) in the Molecular Biophysics and Integrated Bioimaging Division at the Lawrence Berkeley National Laboratory, CA, USA.

## Mark Spackman

Emeritus Professor Spackman is well known around the world for his development of tools and methods from computational chemistry to inform aspects of modern crystallography, especially intermolecular interactions and crystal packing. These research tools have been implemented in the *CrystalExplorer* software package, now used by thousands of students and researchers worldwide. Mark is an emeritus professor at the University of Western Australia (UWA) in Perth, where he received his PhD in 1980. Following postdoctoral stints with R. F. Stewart (Pittsburgh), E. N. Maslen (Perth) and B. M. Craven (Pittsburgh), and an academic appointment at the University of New England (NSW, Australia), he returned to UWA in 2004. In 2013 he was a joint recipient with Carlo Gatti (Milan) of the Gregori Aminoff Prize for Crystallography by the Royal Swedish Academy of Sciences and was awarded the Lawrence Bragg Medal of the Society of Crystallographers in Australia and New Zealand in 2017.

The confirmation of the three plenary speakers and a strong scientific program are sure to elevate IUCr 2023 to new heights.

## Deadline looming for IUCr 2023 abstract submissions

With abstracts already being received, it is clear that IUCr 2023 will be the premier destination for researchers and industry partners in 2023.

The scientific work of the IUCr is conducted primarily through its Commissions. There are 22 individual Commissions and Committees that comprise groups of scientists representing the key areas of crystallography sciences including the following:

Aperiodic Crystals

Inorganic and Mineral Structures

Biological Macromolecules

Magnetic Structures

Committee on Data

Mathematical and Theoretical Crystallography

Crystal Growth and Characterization of Materials

Neutron Scattering

Crystallographic Computing

NMR Crystallography and Related Methods

Crystallographic Teaching

Powder Diffraction

Crystallography in Art and Cultural Heritage

Quantum Crystallography

Crystallography of Materials

Small-Angle Scattering

Diffraction Microstructure Imaging

Structural Chemistry

Electron Crystallography

Synchrotron and XFEL Radiation

High Pressure

XAFS

It is the strong desire of the organising committee to create an inclusive culture and diverse environment at IUCr 2023, which we believe starts with the formation of the academic program, and representatives from each of the Commissions above participated in the IUCr 2023 International Program Committee meeting in April 2022. We encourage you all to submit an abstract, share your knowledge and collaborate with the global crystallography community.

The Call for Abstracts is currently open until **21 November 2022**, with early bird registration available up to **15 February 2023**.

## IUCr 2023 on the move

It was our privilege to be at ACA2022, the 72nd Annual Meeting of the American Crystallographic Association in Portland, OR, USA, the first face-to-face ACA meeting since the pandemic. The excitement and appetite for an IUCr Congress in Australia was palpable. We met over 500 crystallography friends, many of whom were first-time attendees and many of whom were just grateful for the opportunity to reunite. Daily prize draws were conducted, with the final draw being a complimentary registration to IUCr 2023. This ultimate prize was awarded to Samantha Hartanto from the University of California Davis. Thank you to the ACA for hosting us in Portland; what a fantastic city and what a terrific event.




Left: PCO Emma Bowyer and IUCr President Hanna Dabkowska at the IUCr 2023 booth at ACA2022. Right: Samantha Hartanto, winner of a complimentary registration to IUCr 2023.

IUCr 2023 also felt very welcome at the 33rd European Crystallographic Meeting (ECM33) in Versailles, France, and we sincerely appreciate the efforts of the organisers. We had a wonderful and productive time. The start of ECM33 was directly aligned with the launch of the IUCr 2023 Call for abstracts announcement. Our team met over 350 attendees from across Europe and for one of them, the meeting proved extra worthwhile. Congratulations go to Jake Weatherston from Newcastle University, UK, the winner of the complimentary registration to IUCr 2023. The IUCr 2023 stand was enthusiastically depleted of all 'I love Melbourne' koalas, Melbourne-inspired keep-cups and the rare packets of Tim Tams.



IUCr 2023 organizing team members David Aragão, Emma McPartlan and Helen Maynard-Casely at their booth at ECM33 (left), joined by IUCr Promotions Officer Andrea Sharpe and IUCr Journals Editor-in-Chief Andrew Allen (right).

The next stop for the Melbourne team will be the 17th International Conference of the Asian Crystallographic Association in Jeju, Korea.

## Industry support is strong as diamonds

Since our last communication, Rigaku has been confirmed as a Diamond Sponsor for the Melbourne Congress in 2023, joining Bruker and Eldico. There will be many ways for our sponsors and exhibitors to connect with the IUCr community. Our focus is on elevating the delegate experience through the sponsorship of our wellness zones, childcare programs, juice bars and – of course – coffee carts!

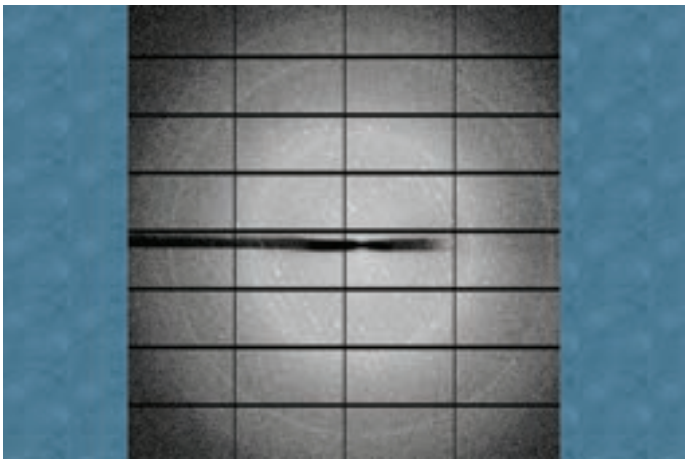
## Accommodation abodes

The Congress team has been busily investigating a range of accommodation choices, from the best hotel facilities to backpacker hostels, with guaranteed room blocks for our IUCr delegates, including students and families.

If you have never been to Australia, it is worthwhile knowing that we have no added taxation at the point of sale. The advertised price is the final price you will pay. We also don't have bed tax here! You can book directly via the website at any time. Alternatively, reach out to our accommodation team if you have an enquiry. Australia's tax-free shopping is called the Tourist Refund Scheme (TRS), which allows overseas visitors and Australian residents to claim a refund of the Goods and Services Tax (GST), so save your receipts and claim at the airport upon departure.

IUCR JOURNALS NEWS

# IUCrData launches Raw Data Letters



L. M. J. Kroon-Batenburg, J. R. Helliwell, J. R. Hester

*IUCrData*, the peer-reviewed open-access data publication from the International Union of Crystallography (IUCr), is launching a new section – Raw Data Letters. This is a collaborative innovation of IUCr Journals with the IUCr Committee on Data. Future raw data sets will become increasingly large and no one group will be able to analyze all of the scientific content in a timely manner. As already occurs in other scientific disciplines (*e.g.* astronomy, particle physics) others will need to have access to raw crystallographic data sets so that open-science-based research can proceed at a rapid pace. However, proper credit needs to be attributed fairly among those who design experiments and collect data, and those who subsequently use the data to establish new results.

With these points in mind, the new section will publish short descriptions of crystallographic raw data sets from X-ray, neutron or electron diffraction experiments, in the biological, chemical, materials science or physics fields, and provide a persistent link to the location of the raw data. The letters in this section will describe interesting features in raw data sets, allowing researchers to attract attention to particular aspects of the data that could be of interest to methods and software developers for purposes such as reanalysis by newer methods or may be relevant to the structural interpretation. We envisage different types of Raw Data Letters. The structure could have been solved and published elsewhere, but the letter describes interesting features that were observed but ignored in the original structure determination. The letter could describe remarkable features but no attempt is made as to their interpretation; in this way the data attract attention and the original authors get credit for their work. The raw data described in a letter show Bragg reflections to a reasonable resolution but the structure could not be solved. Again the authors would get credit for their work. Also letters describing the reuse of publicly available data by improved methods are welcome. In general, publication in Raw Data Letters promotes data retrieval by other scientists and will enhance visibility of the data. Raw Data Letters support Open Science policies: no research data should be lost but should be made available to the research community according to the FAIR principles, for which the correctness and completeness of the metadata are crucial, and these will be central to the reviewing process.

Science funders and policy makers are working increasingly towards the Open Science model to make science useful for society. Good scholarship demands openness and transparency of protocols and scientific results as well as proper data management and validation of scientific knowledge. Many open science platforms have seen the light, *e.g*. the OpenAIRE project (https://www.openaire.eu) and the European Open Science Cloud (EOSC, Jones, 2015) promoting the sharing of data. Guidelines for proper data management are described in *The FAIR principles for scientific data management and stewardship* by Wilkinson *et al.* (2016), which requires research data to be Findable, Accessible, Interoperable and Reusable.

What does this mean for crystallographic data?

*Findable*: the data are assigned a persistent identifier, they come with metadata by which they are indexed in a searchable resource.

*Accessible*: the data should be retrievable through well established communication protocols.

*Interoperable*: the data use a shared (documented) broadly applicable language for knowledge representation.

*Reusable*: the metadata should accurately describe experimental attributes of the data, and are released with a clear and accessible data usage license. Data formats should be described.

The IUCr has always taken a leading position in data sharing by linking publications to coordinates and structure factors as well as validation reports. In chemical crystallography the checkCIF tool, as part of the submission system, ensures consistency and integrity of the data. Likewise, in macromolecular crystallography a paper describing a crystal structure has to link to the Protein Data Bank (PDB) entry, while the wwPDB deposition system generates a validation report. The IUCr established a working group in 2011 (DDDWG) to address 'the growing calls within the crystallographic community for the deposition of primary diffraction images, with some mechanism that allows their retrieval by other scientists for such purposes as reanalysis, software and methods development, validation and review' (see https://forums.iucr.org/). The final report of the DDDWG made a series of recommendations, the first two of which are as follows.

Authors should provide a permanent and prominent link from their article to the raw data sets which underpin their journal publication and associated database deposition of processed diffraction data (*e.g.* structure factor amplitudes and intensities) and coordinates, and which should obey the 'FAIR' principles, that their raw diffraction data sets should be Findable, Accessible, Interoperable and Re-usable (https://www.force11.org/group/fairgroup/fairprinciples).

A registered Digital Object Identifier (DOI) should be the persistent identifier of choice (rather than a Uniform Resource Locator, URL) as the most sustainable way to identify and locate a raw diffraction data set.

The coordinating and advisory role of the DDDWG has been continued by the Committee on Data (CommDat), which was established by the IUCr in 2016. This committee plays a significant role in the current initiative.

A series of papers appeared in *Acta Cryst. D* in 2014 (Guss & McMahon, 2014; Kroon-Batenburg & Helliwell, 2014; Terwilliger & Bricogne, 2014; Meyer *et al.*, 2014) discussing the possibilities of raw-data depositions either in centralized facilities or distributed repositories. Whereas at that time the possibilities of data transfer and estimated costs of storage and curation were seen as a barrier, in recent years several freely accessible repositories have become available that make routine raw-data deposition feasible, and the bandwidth of internet connections has also increased substantially. A recent editorial from IUCr journals (*FAIR diffraction data are coming to protein crystallography*, Helliwell *et al.*, 2019) encourages authors to provide a DOI for their original raw data when submitting their article.

In a topical review in *IUCrJ* (Kroon-Batenburg & Helliwell, 2014), the requirements for metadata are discussed. Without correct and complete metadata we would certainly not adhere to the FAIR principles as the reusability would be compromised.

We also note and have warmly welcomed the PDBj initiative in 2021 to launch its own raw diffraction data archive (https://xrda.pdbj.org/), which is integrated with PDBj, and which opens up the FAIR principles and data record right back to the time of measurement in a depositor's research studies.

With Raw Data Letters we want to elicit re-use of the original data. Diffraction data can be from various disciplines: macromolecular crystallography, chemical crystallography, XFELs, synchrotron serial crystallography, materials science powder diffraction *etc*. These come with many different data formats

and varying metadata quality. To ensure reusability, metadata should be accurate and complete and at least sufficient. For single-crystal data we have made a list of core metadata; their presence is a key requirement for correct (automated) reprocessing of the data. Our list is a superset of the NeXus/HDF5 NxMx Gold Standard that was developed by Bernstein *et al.* (2020). We decided to capture metadata in imgCIF (Bernstein & Hammersley, 2005; Hammersley *et al*., 2005), which is well known to the community via its CBF variant, and already includes the appropriate data names for our core metadata list (see Table 1). imgCIF also has the advantage of being a plain-text format, which allows editing with familiar tools and provides excellent guarantees of readability over the long term.

Table 1. Core metadata list and their data names in imgCIF

| Minimal metadata | imgCIF data name |
| --- | --- |
| Data binary format | _array_structure.byte_order, _array_structure_compression_type, _array_structure.encoding_type |
| Number of pixels, pixel size (binning mode) | _array_structure_list.index _array_structure_list.dimension _array_structure_list_axis.displacement_increment |
| Beam center (mm) | _axis.offset[1..3] (needs _axis category, see below) _diffrn_scan_frame_axis.displacement |
| Origin of data frame | _array_structure_list.precedence (1 or 2) _array_structure_list.direction (increasing or decreasing) |
| Wavelength | _diffraction_radiation_wavelength.value(/wavelength) or _diffraction_radiation.type |
| Rotation axis | _diffrn_scan_axis.axis_id _diffrn_scan_axis.angle_start _diffrn_scan_axis.angle_range |
| Rotation range per frame/number of frames | _diffrn_scan_axis.angle_increment,_diffrn_scan.frames _diffrn_scan_frame.frame_number |
| Axes and offsets | _axis.id, _axis.type, _axis.depends_on, _axis.vector[1] _axis.vector[2] _axis.vector[3] _axis.offset[1] _axis.offset[2] _axis.offset[3] |
| Detector-to-sample distance | _diffrn_scan_axis.displacement_start _diffrn_scan_axis.displacement_range |
| Conditions | _diffrn.ambient_temperature |

The current core metadata list has been specifically developed for single-crystal data; it will have to be extended for powder diffraction and high-pressure data; XFEL data will also need additional information.

There are two aspects to metadata that need attention after having established the core metadata list: (1) we need to generate the metadata from the original raw data format, possibly completed by user-supplied metadata, and (2) we need a checking procedure for checking consistency and correctness that can be used on the IUCr webserver.

A separate working group has been developing tools for extracting metadata information from raw images. A key problem is that raw data, unlike structural data, may be deposited in one of a multitude of formats currently in use. The situation for large-scale facilities is somewhat different to that for home diffractometers. Large-scale facilities often have PILATUS detectors that use CBF binary data format and miniCBF (ASCII) headers or EIGER detectors that use the Nexus/HDF5 data structure; at the same time CCD detectors may still be in use. Home diffractometers often have manufacturer-developed detectors and binary image formats. Most home diffractometers also have multi-circle diffractometers that make the description of metadata more complicated.

Practical issues have forced us to compromise on the DDDWG recommendations above. We have adopted an approach where the metadata, in the form of an imgCIF file, is separated from the raw data frames, to avoid the need for unfeasibly large data downloads during the validation process. The imgCIF file required during submission instead contains internal pointers to the raw data as URLs. The use of URLs, rather than more robust DOIs, is an additional compromise resulting from the requirement that checks be able to access the actual data files containing the data frames; there is no standardized way of finding the data files from data DOIs as the DOI usually resolves to an informational 'landing page'. To mitigate against the URL fragility that DOIs were designed to avoid, the accessibility of all repositories referenced by archived imgCIF files held by the journal will be regularly checked, and in the rare case that URLs become inaccessible they will be manually updated using the data DOI provided by the authors during submission. Once the data DOI specifications mature to the point that data files can be directly referenced, our approach envisages that the URL form of a data DOI would be used in the submitted imgCIF file. We understand that our solution is necessarily a compromise, and will continue to refine the way in which raw data are handled as we gain experience and receive feedback from the community.

For the first letters published, we generated complete and consistent imgCIF files using the CBF laboratory axis system. For the macromolecular letter (Neviani *et al.*, 2022), we used a Python script written by Fabio Dall'Antonia and Julian Hörsch (European XFEL) to convert the metadata information from a Nexus/HDF5 master file into CBF/imgCIF. This particular Diamond Light Source Nexus/HDF5 (meta)data follows the 'Gold Standard' defined by the HDRMX working group (Bernstein *et al.*, 2020). The CBF laboratory axis system is different from that of Nexus McStas. Fig. 1 explains the details.

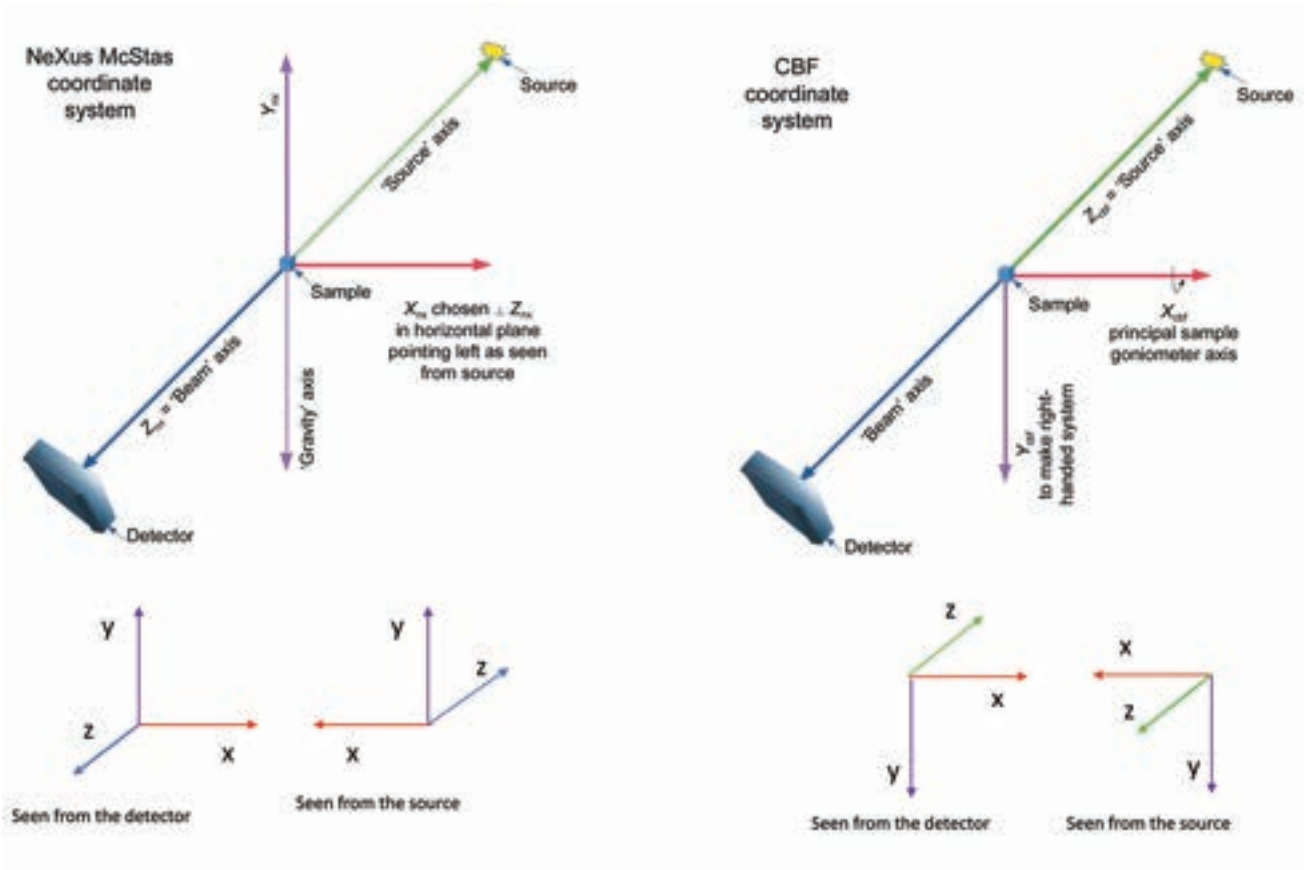



Figure 1. The Nexus McStas axis system is different from the CBF laboratory system. Seen from the source in McStas, *Z* points away from the source and the *X* axis points to the left, while in CBF *Z* points back into the source and *X* is along the principal goniometer axis, *i.e.* points into the goniometer block. A vector defined in McStas is brought by a 180° rotation around Nexus_X to the CBF system. Note that if the goniometer is at the opposite side, the transformation is around Nexus_Y (image courtesy of the Gold Standard paper, Bernstein *et al.*, 2020).

Most diffractometer manufacturers provide software for conversion to CBF, mostly miniCBF headers and CBF binary data. Bruker AXS was very helpful in providing a tool for image conversion to full CBF files. We used these files as the basis for our imgCIF file in the letter describing the twinned form of *o*-nitroaniline (Lutz & Kroon-Batenburg, 2022).

Procedures and tools for the generation of imgCIF files from the available image data files are being incorporated into the IUCr Journals submission system. This is ongoing work, as we have to deal with many different formats, and contributions from the community are welcome. Further information on tools for authors will available shortly.

Submissions are now being welcomed – updated Notes for authors and submission instructions are available from the *IUCrData* website. This is early days for the Raw Data Letters section. Our Co-editors (see https://iucrdata.iucr.org/x/services/editors.html) are very keen to work with authors to facilitate publication of their data. We look forward to receiving your Raw Data Letters.

## Acknowledgements

We thank the members of the working group for discussion and constructive contributions to the development of the format of the Raw Data Letters and checkCIF tools: Fabio Dall'Antonia, Julian Hörsch, Andy Götz, Brian McMahon, and the IUCr Journals Editorial Office. We thank Joerg Kaercher (Bruker AXS) for providing a tool for conversion from Bruker sfrm format to full CBF, and for fruitful discussions.

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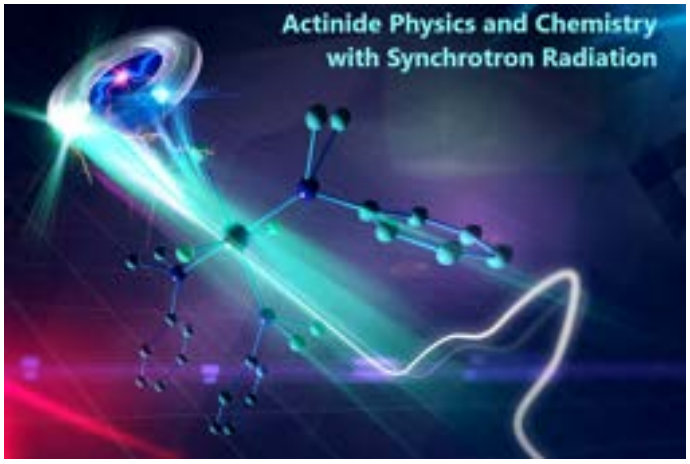
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IUCR JOURNALS NEWS

# Foreword to the special virtual issue on Actinide physics and chemistry with synchrotron radiation




Kristina O. Kvashnina, Sergei M. Butorin, Shuao Wang, Weiqun Shi

Actinide research is currently experiencing a renaissance in the fields of material science, nanotechnology, medicine and environmental science. It is now possible to study the chemistry and physics of the actinide elements (all radioactive) using state-of-the-art non-destructive techniques at synchrotrons which have not been available before. The beamlines and instruments dedicated to actinide research have made various spectroscopic and scattering methods accessible to scientists worldwide. The new synchrotron sources at the large-scale facilities offer more advanced possibilities for the development of new methodologies in actinide science in the future. Theoretical studies of actinides are followed by unique experimental methods and novel experimental data.

The virtual special issue on *Actinide Physics and Chemistry with Synchrotron Radiation* (https://journals.iucr.org/special_issues/2022/actphyschem/index.html) includes several invited contributions that focus on novel results obtained for actinide materials with the help of synchrotron radiation. In total, 19 articles cover a broad variety of synchrotron-based spectroscopic and scattering methods used to study actinide-containing materials and can be tentatively divided into five groups:

(1) Gerry Lander and Roberto Caciuffo reviewed the X-ray diffraction (XRD), resonant X-ray scattering (RXS), X-ray magnetic circular dichroism (XMCD), resonant and non-resonant inelastic scattering (RIXS, NIXS), and dispersive inelastic scattering (IXS) experiments in studies of actinide materials (Caciuffo & Lander, 2021). Advanced synchrotron-based spectroscopic methods, such as X-ray absorption near-edge structure (XANES), recorded in the high energy resolution fluorescence detection (HERFD) mode at the U $L_3$- and $M_4$-edges were used by Sergei Butorin and co-workers in the chemical state investigation of uranium carbides supported by single Anderson impurity model (SIAM) theory (Butorin *et al.*, 2022). Rene Bes and co-authors reported HERFD-XANES data at the U $L_1$-edge of $KUO_3$ analysed by electronic structure calculations (Bes *et al.*, 2022). Tim Pruessmann and co-workers applied the HERFD/RIXS methodology at lanthanide and actinide $L_3$-edges in combination with low-*Z* element *K*-edge XANES along with electronic structure calculations to probe the chemical and physical properties of *f*-electron systems (Pruessmann *et al.*, 2022).

(2) Alexander Scott Ditter and co-authors showed the power of soft X-ray spectromicroscopy at the O *K*-, U $N_{4,5}$- and Ce $M_{4,5}$-edges for spent nuclear fuel investigations, yielding chemical information on the sub-micrometre scale (Ditter *et al.*, 2022). Yusheng Zhang and co-workers investigated the covalency effects in the bonding between the uranyl ion and dithiophosphinate by combining sulfur *K*-edge XANES

and density functional theory (Zhang *et al.*, 2022).

(3) Lin Wang and co-authors combined X-ray diffraction and extended X-ray absorption fine-structure (EXAFS) methods to study thorium(IV) adsorption onto multi-layered titanium carbides, $Ti_3C_2T_x$ (Wang *et al.*, 2021). Jian Sun and co-authors studied two series of uranium-doped $Nd_2Zr_2O_7$ pyrochlore materials as potential nuclear waste host matrices by the combination of the X-ray diffraction, Raman and EXAFS techniques (Sun *et al.*, 2022). Using EXAFS at the U $L_3$-edge and XRD, Antonia S. Yorkshire and co-authors investigated U(VI)–cement mineral interactions, relevant to understanding the waste disposal of actinide-containing materials (Yorkshire *et al.*, 2022). Hao Ding and co-workers examined synthetic Chernobyl lava specimens using micro-focus spectroscopy at the U $L_3$-edge along with diffraction techniques and were able to construct U oxidation state maps (Ding *et al.*, 2021). Anna Krot and co-workers performed U(VI) speciation in contaminated environments using EXAFS data recorded at the U $L_3$-edge on U reference compounds (Krot *et al.*, 2022). Cyril Zurita and co-workers utilized Pu $L_3$ EXAFS to study the interaction of Th(IV), Pu(IV) and Fe(III) with ferritin protein (Zurita *et al.*, 2022).

(4) Thomas Dumas and co-authors studied the size and structure of the hexanuclear plutonium oxo-hydroxo clusters in an aqueous solution by combining small-angle X-ray scattering (SAXS) and Pu $L_3$-edge EXAFS methods (Dumas *et al.*, 2022). Anna Romanchuk and co-workers proposed a new core-shell approach for the actinide and lanthanide dioxide nanoparticles with calculated effective coordination numbers from Ce *K*-edge and Th and Pu $L_3$-edge EXAFS (Romanchuk *et al.*, 2022). Baihui Zhai and co-authors studied the formation and structure of polynuclear thorium(IV) colloids and thorium dioxide nanoparticles by SAXS (Zhai *et al.*, 2022).

(5) Korey P. Carter and co-authors reported on the *in situ* beam reduction of Pu(IV) and Bk(IV) during Pu/Bk $L_3$ XANES/EXAFS measurements, which yielded Pu(III) and Bk(III) coordination complexes with hydroxypyridinone chelators (Carter *et al.*, 2022). Richard Husar and co-workers performed *in situ* Np $L_3$-edge XANES/EXAFS measurements and density functional theory calculations in combination with an electrochemical setup, dedicated to radioactive samples (Husar *et al.*, 2022). Damien Prieur and co-workers conducted *in situ* U $L_3$-edge XANES measurements and thermodynamic calculations to establish the U–O phase diagram (Prieur *et al.*, 2021). Bianca Schacherl and co-authors implemented the cryogenic sample environment for the tender X-ray range, necessary for actinide HERFD $M_{4,5}$-edges data collection on radioactive samples (Schacherl *et al.*, 2022).

There is no doubt that synchrotron radiation plays a critical role in understanding the physics and chemistry of actinide-containing materials. We very much look forward to continued developments in experimental and theoretical synchrotron-based methodologies for fundamental and applied actinide science in the future.

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EDITORIAL

# Model building and beyond




The cover illustration for the CCP4 Study Weekend 2020 special issue, shown above, is a creative work that shows how solving a new structure is like an adventure, full of riddles and traps. The easier path never shows up the most amazing view of a landscape, like a revelation to human eyes for the first time. By Marco Salamina, Newcastle University, UK.

Jon Agirre, Robbie P. Joosten, Alan Roseman

The three main macromolecular structure determination techniques are different enough to hold separate congresses and reunions, but there is one topic that connects them like no other: everyone wants to build the best possible atomic model. The 2020 CCP4 Study Weekend, held 7–9 January 2020 in the East Midlands Conference Centre (Nottingham, UK) while COVID-19 was still an outbreak on the other side of the globe, revisited this topic with integrative spirit.

For the first time ever, the meeting opened with a tag-team talk. Eleanor Dodson and Helen Saibil gave a historic perspective and introduced the particularities of model building in macromolecular X-ray crystallography and electron cryo-microscopy (cryo-EM), respectively. The meeting, cross-discipline by design, continued with a session on automated model building, opened by Tom Terwilliger, who discussed his methods for interpreting and improving cryo-EM maps automatically. The session continued with Isabel Usón, who is taking the mantle from George Sheldrick on the development of *SHELXE* and is adapting the software to trace models with maps calculated from electron diffraction data. Kevin Cowtan closed the session with a provocative talk on competitive versus collaborative science, based on their comparison of model building packages, presented in this special issue.

Once a model is obtained, it is time for real or reciprocal space refinement, hence our next session covered several methods for model correction and improvement. Garib Murshudov compared the particularities of X-ray crystallography and cryo-EM maps, laying the foundation for the next talk by Dorothee Liebschner, who discussed methods for automatic refinement of models in cryo-EM maps. Ana Casañal and Tristan Croll presented the latest improvements in real-space refinement in the *Coot* and *ISOLDE* software respectively, with Hamish Todd taking 3D model building to the next level through an exploration of the possibilities and limitations of virtual reality (VR) hardware for interactive model building.

While building a protein can be done fully automatically in an ever growing number of cases, identifying and building ligands is comparatively still a bottleneck due to the absence of a reference sequence, generally poorer density, the potential for multiple binding modes, or the very human self-deception in cases where there is no binding. Mihaela Atanasova discussed the York methods for carbohydrate model building, refinement, validation and analysis. Antonio Rosato covered metals, their coordination and

representation in the MetalPDB database. Robert Nicholls offered solutions to the challenges posed by the building and refinement of covalently attached ligands and modifications, such as enzyme–substrate intermediates or protein glycosylation, respectively. Rachael Skyner presented the *Fragalysis* open source software, which allows the user to closely inspect numerous structures of protein–ligand complexes, all stored in the cloud and represented in a web browser. Dinner and the traditional ceilidh followed, paving the way for one of the last traditional social occasions in two years, as the 2021 and 2022 Study Weekends were remote-only events due to the COVID-19 pandemic.

The second day began with a session on low-resolution model building, led by Agnel Joseph who discussed flexible fitting and other tools in *Flex-EM*. Valeriy Titarenko presented methods for the identification of fragments in low-resolution cryo-EM reconstructions, adapting functions traditionally used in crystallographic molecular replacement. Helen Ginn introduced the *Vagabond* refinement software, where molecules are refined in torsion angular space. Sarah Harris explained how molecular dynamics can help even in projects where large molecular size can be a problem.

The next two sessions covered protocols and tools to use whenever a model is nearing deposition: validation, analysis and representation were brought into the foreground. Wah Chiu presented the results from the EM validation challenge; while most tools for model validation are easily transplantable from X-ray crystallography, certain problems are particular to EM and need dealing with as the average resolution of EM structures keeps improving. John Berrisford gave an overview of the tools and procedures associated with protein structure deposition in the Protein Data Bank in Europe and beyond – John was also a driving force behind the deposition tools in both *CCP4i*2 and CCP4 Cloud interfaces. Jiří Černý discussed methods for the validation of nucleic acid structures which, very much like saccharides in general, are of paramount importance to biological structures but have been left behind in method development in favour of a protein-centric perspective. Rafiga Masmaliyeva presented *toBvalid*, a tool for the analysis and validation of temperature factors. In the next session, but largely under the same topic, Anastassis Perrakis gave an overview of the validation and model improvement services in *PDB-REDO*. Marc Baaden showcased his software for the representation and analysis of macromolecules in VR in another example of gaming technology aiding scientists. David Sehnal concluded the session offering an overview of *Mol**, the default molecular webviewer used by the PDB websites.

The meeting concluded with a mesmerizing talk by Jeroen Claus of Phospho Ltd, who demonstrated the application of industry-standard 3D modelling tools to the high-end visualization of macromolecular atomic structures.

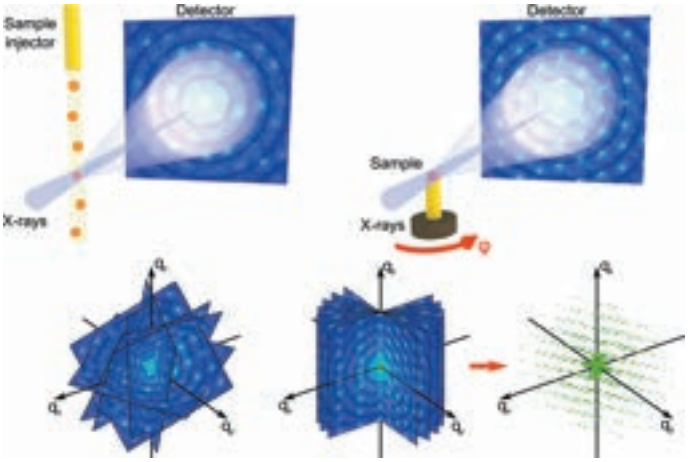
The cover competition, which ran for the first time in the 2020 Study Weekend, produced a number of high-quality submissions. The winner of the contest, Marco Salamina's 'Structural Biology: the lost structure', is showcased on the cover of both the virtual and printed editions, as well as the graphical abstract for this introduction.

We are grateful to CCP4 and its people for funding, championing and running the meeting. And, more than ever, we would like to acknowledge the work all the speakers put into their well crafted talks and carefully prepared papers for this proceedings issue, which is available as a virtual issue at https://journals.iucr.org/special_issues/2020/CCP42020/, and is now complete after a two-year winter.

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COMMENTARY

# Going beyond ensemble average angular cross-correlation analysis




Espen Drath Bøjesen

Analysis of angular correlations of scattering intensities has, albeit initially only sporadically, been used as a tool for studying materials structure dating back to the 1970s (Kam, 1977; Clark *et al*., 1983). However, since the seminal work by Wochner *et al*. (2009), angular cross correlation analysis (ACCA) has experienced somewhat of a renaissance due to advances in instrumentation and computing power. The advent of third- and fourth-generation synchrotron sources, free-electron lasers, modern electron microscopes, novel detector technologies, and improved computing capabilities have led to a renewed interest in ACCA. Recent studies include expansion of the underlying theory (Altarelli, 2010; Martin, 2017) and a plethora of examples where ACCA has been central to revealing novel insights into, for example, the mechanical stability of colloidal glasses (Liu *et al.*, 2022), the structural nature of metallic glasses (Liu *et al.*, 2013), defects in disordered carbons (Martin et al., 2020), and even protein structures (Adams *et al*., 2020).

In the current issue of **IUCrJ**, Lapkin *et al.* (2022) propose a novel application of ACCA – namely expanding its applicability to facilitate analysis of single-crystal X-ray scattering data collected from colloidal single crystals. This tactic breaks with more commonly adapted approaches to ACCA, which rely on collecting vast amounts of X-ray or electron scattering patterns from randomly oriented individual samples or from multiple different locations in one individual sample (possible with scanning X-ray or scanning electron scattering approaches). Both these tactics assume that by collecting enough individual scattering patterns the entire 3D reciprocal space volume will be sampled. This notion is reasonable for structurally homogeneous samples without any significant degree of preferred orientation, such as glassy materials, but may fail for more ordered samples.

The new scheme devised by Lapkin *et al.* avoids the need for complex iterative phase-retrieval algorithms while still providing critical qualitative insights to the real-space structure of a single-crystalline grain. By studying individual crystals, insights into potential structural variations across a sample (*i.e.* a collection of crystals from a 'synthesis') may be accessed. This contrasts previous ACCA of scattering data, which generally provides insights into ensemble average structure. The original methodology thus facilitates *quick-and-easy* assessment of structural features in colloidal crystals. In the paper, Lapkin *et al.* nicely demonstrate the feasibility of their approach by presenting analyses of both simulated as well as experimental X-ray scattering data to reveal various types of stacking disorder in colloidal crystals. The ability to easily judge the type and approximate concentration of such defects is where this method really excels.

The addition of this tool to the ever-expanding toolbox of scattering-based structural analysis is a timely reminder of the importance of considering the differences between studies of the ensemble average structure of a sample and studies of spatial variations of local structure in a sample. Within the field of X-ray scattering (not counting single-crystal studies) there has been a tendency to focus on the former to provide important structural insights with impressive statistical significance. This statistical potency, however, inadvertently comes with a lack in sensitivity towards often property defining manifestations of structural heterogeneity. Similarly, methods that only study very small sample volumes, *e.g.* electron microscopies, lack the statistical gravitas of ensemble average methods. As previously mentioned, vast improvements in experimental capabilities now finally enable detailed studies of structural heterogeneity at multiple length scales. Along these lines, there lies great potential in exploring the combination of the methodology from Lapkin *et al.* with already established 'ensemble average' based ACCA techniques to get *the best of both worlds.*

Finally, the proof-of-concept study presented by the authors opens attractive new avenues. For one, the newly established tactics can be used in their current state to reveal the structural origin of relevant materials problems – including *in situ* or *operando* studies. Furthermore, expanding the capabilities of the presented analysis approach to apply to structures of other length scales than colloidal crystals is an exciting direction for the community to explore. For example, it would be interesting to investigate the possibility of studying assemblies of nanosized (2–4 nm) atomic clusters into hierarchical structures or even the atomic structure of nanosized single crystals by adapting the method from Lapkin *et al*. to be suitable for analysis of electron scattering data.

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COMMENTARY

# Solving molecular compounds from powder diffraction data: are results always reliable?

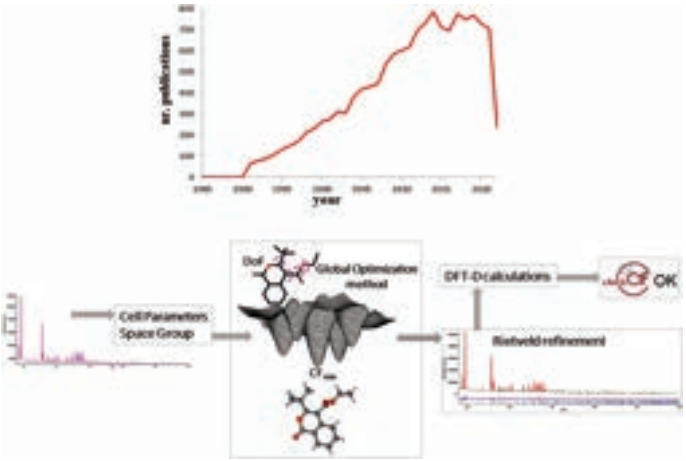



Figure 1. Progress in structure solution from PXRD data. (Top) Approximate numbers of publications involving structure solution from powder diffraction (source: Web of Knowledge search, June 2022). (Bottom) Steps of a crystal structure solution process from PXRD through global optimization methods.

Angela Altomare

Powder X-ray diffraction (PXRD) is a powerful tool for solving microcrystalline powder structures. Writing in **IUCrJ**, Schlesinger *et al.* (2022) report intriguing results demonstrating that, in the case of poor-quality PXRD data, starting from one experimental pattern, we can obtain different structure solutions, all crystallochemically plausible and satisfying the reliability criteria currently adopted in the solution process. This unexpected situation suggests adopting a more critical attitude towards structure determination from powders.

Crystallographic study is the leading scientific approach for recovering unambiguously the arrangement of atoms in a crystalline system. In the case of a single crystal, the structure determination is rarely affected by errors because the quality of the experimental diffraction data is usually good. However, in the powder case, the structural study faces several, and often concurrent, problems due to peak overlap, background noise, preferred orientation, limited quantity, poor quality of diffraction data, *etc.* Nevertheless, structure solution from powders has registered an increasing success over the years (*cf.* Fig. 1). Thanks to valuable methodological advances and high-performance computational resources (David, 2019; Altomare *et al.*, 2019; Černý *et al.*, 2019; Gilmore *et al.*, 2019), we are now able to quite easily solve small molecular structures, especially if Bragg peaks in the diffraction patterns are sharp and the background noise is low. In particular, global optimization (GO) methods have become very popular to the point that they are sometimes preferred to direct methods, even when the latter can be successfully applied. In addition to the determination of unit-cell parameters and space group, the solution process through GO methods requires comprehension of the expected molecular geometry. The GO methods randomly move a starting structure model around the cell, in accordance with the assumed symmetry, adjusting its position, orientation and conformation (degrees of freedom, DoF) with the aim of reaching the global minimum of a cost function (CF, based on agreement between the observed and calculated profiles) and providing the correct solution. The solution process is completed by Rietveld refinement, followed by a careful crystallochemical check of the structure solution. Validation with dispersion-corrected density functional theory (DFT-D) calculations is recommended (van de Streek & Neumann, 2014). Finally, the corresponding CIF (crystallographic information framework) file is

submitted to a crystal structure database (*cf.* Fig. 1).

Schlesinger *et al.* focus their PXRD investigation on the unknown crystal structure of 4,11-difluoro-quinacridone ($C_{20}H_{10}N_2O_2F_2$, DFQ), a non-commercial organic pigment derivative of quinacridone. With a rigorous and deep analysis, they prove that the DFQ structure is ambiguously solved if the solution process is carried out by a GO method followed by Rietveld refinement. At the same time, they demonstrate that a suitable combination of complementary methods can overcome this ambiguity and move towards the correct solution.

The DFQ poor-quality experimental diffraction pattern, collected on a laboratory X-ray powder diffractometer, presents only a few sharp and some broad Bragg peaks with severe overlap. Owing to a low level of crystallinity, the inadequate quality of this pattern cannot be improved upon by using synchrotron radiation. As things stand, the determination of unit-cell parameters by the most widely used indexing software is unattainable and the structure solution of DFQ can be classified as challenging.

Schlesinger *et al.* try to solve the DFQ structure by using the GO-based computing program *FIDEL-GO* (Habermehl *et al.*, 2022), which has been specifically developed for structure determination from unindexed data. The rationale of *FIDEL-GO* is the global fit between simulated and experimental powder data: about 21 million random starting structure models compatible with the expected molecular geometry, located in cells with random parameters and different space groups, are submitted to the optimization process; unit-cell parameters, molecular position and orientation, and selected internal DoF are fitted simultaneously to the powder pattern; a similarity measure based on cross-correlation functions allows the comparison of simulated and experimental data. An automatic Rietveld refinement, a DFT-D geometry optimization and a user-controlled Rietveld refinement complete the solution process.

Four crystallographically different solutions, all worthy of being published, are obtained thus making uncertain the principle of structure unambiguity: they are all chemically reasonable (check of molecular packing, intermolecular distances, short intermolecular contacts); they are all compatible with the experimental diffraction pattern, and they surprisingly end with acceptable low *R*-values from Rietveld refinements; they all pass the *CheckCIF* test with trivial alerts. From an extensive examination of topology and Rietveld fits, only a slight preference for two of the solutions comes to light. Which one of them is correct?

Examples of incorrect published structures and structure ambiguity from PXRD are reported in the literature, but Schlesinger and colleagues go beyond this and accomplish a comprehensive analysis of the four structure candidates. They accurately compare the candidates and disclose why they are all compatible with the same experimental profile. Moreover, they reveal structure disorder by inspecting peak broadening.

It is significant that the authors solve the crux of ambiguity with the aid of additional analyses: (*a*) intramolecular and intermolecular examination through extensive pair distribution function (PDF) refinements (Schlesinger *et al.*, 2021) using synchrotron data collected at both room temperature and 173 K; (*b*) evaluation of colour; (*c*) lattice-energy minimizations using force fields (Dassault Systemes, 2008) by optimizing molecular geometry and lattice parameters; (*d*) lattice-energy minimizations by DFT-D (Neumann *et al.*, 2008; Giannozzi *et al.*, 2017) by optimizing atomic positions and lattice parameters and calculation of the root mean square Cartesian deviation (RMSCD) of non-hydrogen atoms (van de Streek & Neumann, 2010); (*e*) solid-state NMR study with measurements of $^{13}C$, $^{1}H$ and $^{19}F$ spectra.

Overall, this insightful study reveals that structures solved from limited-quality PXRD data can be questionable if not supported by a multi-methodological solution strategy, as well as providing the correct structure of DFQ. The authors interestingly demonstrate that the application of the PDF fit method for structure refinement is promising.

A reasonable question arises from this work: can the combination of methods applied by Schlesinger *et al.* be generalized? Does this combination remove ambiguity in other similar cases? The issue remains

open.

*The answer to the question in the title is yes, even in the case of low crystallinity, but a critical inspection of results must be carried out every time the solution process is executed by using methods based only on the best fitting of the experimental PXRD pattern.*

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REGIONAL NEWS

# Celebrating 50 years of European crystallography in Versailles




Left to right: Bill Clegg (Perutz Prize), Éric Collet (Kálmán Prize), Lukáš Gajdos (2022 Bertaut Prize) and Ellen Fogh (2021 Bertaut Prize).

Arie van der Lee

Although the COVID-19 pandemic is not yet completely behind us, European crystallographers started to meet again in person in 2022, taking advantage of a relatively calm COVID period during the summer. The scientific highlight of the European Crystallographic Association (ECA) was this year the gathering of 805 delegates and 78 exhibitors at the 33rd European Crystallographic Meeting from 23 to 27 August in Versailles, France. The scientific program comprised a dense mixture of topics in 47 microsymposia through all branches of crystallography. Two public lectures were devoted to the local French context: one on the life and work of René-Just Haüy, one of the founding fathers of modern crystallography who died 200 years ago in Paris, and the other one on the scientific aspects of the renovation of the Notre Dame cathedral in Paris that burned heavily in 2019.

The meeting also saw three ECA prizes awarded: the Perutz Prize went to Professor Bill Clegg (Newcastle University, UK), the Kálmán Prize to Professor Éric Collet (University of Rennes, France) and the Bertaut Prize to Dr Lukáš Gajdos (Institut Laue-Langevin, Grenoble, France). The 2021 Bertaut Prize was awarded this year as well; Ellen Fogh from the EPFL in Lausanne, Switzerland, was the lucky awardee but received the prize at the International Conference on Neutron Scattering in Argentina.

This year European crystallographers celebrate the foundation of the European Crystallographic Association 25 years ago in Lisbon, Portugal. It succeeded the European Crystallographic Committee (ECC) that was founded exactly 50 years ago in 1972 in Bordeaux, France, at the very first European Crystallographic Meeting. We had the pleasure to welcome in Versailles not only all Past Presidents of the ECA except one but also one of the founding fathers of the ECC and ECA, Paul Beurskens (Nijmegen, the Netherlands), who despite his 88 years is still remarkably lively. Paul and the Past Presidents, together with Bill Clegg representing ECA’s senior crystallographers and Philipp Hans representing ECA’s young crystallographers, presented their views and highlights of European crystallography during a special ceremony.




From left to right: Marijana Đaković, Andreas Roodt, Hartmut Fuess, John Helliwell, Santiago Garcia-Granda, Claude Lecomte, Philipp Hans, Alessia Bacchi, Udo Heinemann, Bill Clegg and Paul Beurskens.



Many delegates had dinner together during a magnificent boat trip on the Seine river, straight through the heart of Paris, underneath the Eiffel Tower and the Notre Dame cathedral.

The ECA Executive Committee continued working on different topics, at physical meetings in Zagreb (29–30 April) and during two meetings in Versailles, but of course also very often remotely. Since the adoption of new statutes by the Council in 2021, we aim to obtain charity status in the Netherlands where the ECA is registered for two reasons: the charity status will put the ECA on safe legal ground in

terms of its charitable and tax status and it will create the tax and legal framework for the transfer of the Perutz–Bertaut funds from Darmstadt to the ECA. A new treasurer was elected during the Council Meeting: Antonia Neels from EMPA and the University of Fribourg, Switzerland. Antonia succeeds Jacob Overgaard who decided to make a turning point in his career. We thank Jacob for serving the ECA for four years. The Council also approved a bid from Nancy, France, to organize the 9th European Crystallographic School (ECS9) in 2024, which will follow ECS8 in Berlin, Germany, in 2023, and ECS7, which was held in Lisbon, Portugal, in July of this year.

European crystallographers continue to meet during the ECA's monthly lunchtime webinars, a successful series covering all sub-disciplines in crystallography and organized by the ECA's young crystallographers. The next in-person large international crystallographic meeting will be the 26th IUCr Congress in Melbourne, Australia, in 2023. About 10 Australians were present at ECM33 in Versailles; hopefully we will see a lot of Europeans travelling Down Under next year! ECM34 will take place in Padova, Italy, from 26 to 31 August 2024 and will be followed immediately at the same venue by EPDIC18, the 18th European Powder Diffraction Conference: a truly good opportunity for all European crystallographers to meet!

CRYSTALLOGRAPHY IN AFRICA

# The Senegalese Crystallography Association: the walk towards its creation

Ibrahima El Hadji Thiam, Patrice Kenfack Tsobnang, Magatte Camara

The United Nations declared 2014 the International Year of Crystallography (IYCr) under the initiative of the IUCr, spearheaded by the Moroccan Crystallographic Association. One main activity during the celebration of this IYCr was the Pan African Summit meeting held from 15 to 17 October 2014 at the University of the Free State, Bloemfontein, South Africa. This summit meeting was organized with the view of shining a spotlight on crystallography in Africa. The President of the IUCr, the Director of Science Policy and Capacity Building Division in UNESCO, the President of the European Crystallographic Association (ECA), the Commissioner of Human Resources, Science and Technology: Africa Union, and several African government ministers of Science and Technology, Higher Education, Scientific Research and Education, requested through a letter the initiation and support of actions to promote crystallography in Africa. The promotion of crystallography envisaged at the IYCr summit is facilitated through the involvement of the African Crystallography Association (AfCA), and also through national Crystallography Associations within the continent. In this article, we outline the actions that led to the launch of the Senegalese Crystallography Association (SCA). The vision, objectives and founders of this youngest Crystallography Association in Africa are also presented.

## Actions leading to the launch of SCA

## Schools organized in Senegal

Two Schools on Crystallography were organized in Ziguinchor, Senegal, as part of the framework of the IUCr Africa Initiative chaired by Professor Claude Lecomte (University of Lorraine, Nancy, France).

The first School was a Travelling Lab organized from 5 to 10 October 2015 at the Assane Seck Ziguinchor University (UASZ). This first School on crystallography in Senegal had 45 participants, mostly from Senegal, but there were also participants from Benin, Burkina Faso, Ivory Coast and Madagascar. Of the participants, 65% were Masters or Doctoral students from departments of chemistry, physics or pharmacy.




Participants in the first Travelling Lab at UASZ.

The main objective of the School was to allow young researchers, university teachers and engineers from Africa to acquire basic knowledge in X-ray diffraction and crystal structure determination through lectures and supervised tutorials. This was achieved thanks to lecturers from France and Cameroon, and the organizing committee chaired by Professor Magatte Camara. The School was supported by UNESCO, IUCr, CCDC and UASZ, as well as Bruker, which provided the diffractometers (X2S and D2 Phaser) used during the School.



Loïc Le Dréau (from Bruker) explaining to the participants how X2S and D2 Phaser work.



Professor Claude Lecomte in discussion with Senegal's Minister of Higher Education and Scientific Research on the necessity of supporting research activities in crystallography, which underpins other sciences.

The second School in Senegal was a Type 1 OpenLab. It was jointly organized by the IUCr, IUPAP, ITCP and the UASZ, and was held from 22 November to 2 December 2017 at Ziguinchor. It brought together 30 participants from 11 countries: Benin, Burkina Faso, Cameroon, Côte d'Ivoire, Congo Brazzaville, Democratic Republic of Congo (DRC), Gabon, Madagascar, Nigeria, Sudan and Senegal. As before, most of the participants were from Senegal.




Participants in the IUCr-IUPAP-ICTP OpenLab at UASZ.

The main objective of this IUCr-IUPAP-ICTP OpenLab, which was to equip each participant with sufficient knowledge of the theory and practice of X-rays, neutron crystallography and synchrotron radiation, was achieved. Topics such as the physics of X-ray and neutron diffraction, powder and single-crystal methods,

physical properties of crystals, symmetry and space groups, structural refinement, crystallographic databases, nanocrystallography, biocrystallography and synchrotron light diffraction applications were discussed during the lectures. The lecturers were from France, Italy, Cameroon and Algeria, and were invited by the scientific committee chaired by Professor Claude Lecomte. Thanks go to the sponsors of the event and the organizing committee chaired by Professor Magatte Camara.

## The teaching and research activities of Senegalese researchers in crystallography

After the two Schools, in view of continuing the training of Senegalese people in the field of crystallography, and to share this knowledge with students, many aspects of this science were introduced into university programmes, and research projects around crystallography were improved. Collaborations with researchers in the field around the world were also established. Many PhD and Masters works in the field were prepared. The number of articles in IUCr journals with at least one author affiliated to an institution in Senegal from 2014 to 2023 (63 articles), compared with the number from 1948 to 2013 (57 articles), is a good illustration of the effect of this promotion of crystallography in Senegal. Also, one member of the AfCA Executive Committee, Dr Mamoudou Diallo, is from the SCA.

## The participation of Senegalese researchers in crystallography conferences

Among the many activities undertaken to continue the training of Senegalese researchers in the field of crystallography, a key aspect is their participation in conferences, workshops, schools etc. Some of the conferences and workshops that researchers from Senegal attended include PCCr1 held in Dschang (Cameroon), PCCr2 in Accra (Ghana), ePCCr, various crystallographic schools organized by $CRM^2$ (France) and the Zürich Crystallography School.



Senegalese delegation to PCCr1 at the University of Dschang, Cameroon.

## The launch of the SCA, its vision and objectives

As a result of the strength of the activities mentioned above, and with the view of transforming all of them into long-term sustainable actions, Senegalese researchers recently proposed the idea of setting up an association open to Senegalese people working in crystallography or interested in the development of Senegal through this science. For this purpose, after many meetings, seven researchers from the UASZ, the University Cheikh Anta Diop of Dakar (UCAD) and the Gaston Berger University (UGB) in Saint Louis created the Senegalese Crystallography Association, and on 12 March 2022, a constitutive General Assembly with 30 scientists was organized. The statutes and by-laws of this youngest African crystallography association were approved, and the association was launched.




Founder members of the SCA.

The composition of the first Executive Committee of this SCA is given below:

**President:** Professor Magatte Camara (UFR ST – UASZ)

**Vice-President:** Professor Rokhaya Guèye Sylla (FMPO – UCAD)

**General Secretary:** Professor Ibrahima Thiam (FST – UCAD)

**General Treasurer:** Professor Mbossé Ndiaye Guèye (UFR SAT – UGB)

The SCA aims to promote Senegal's crystallographic and structural sciences. The Association also wants to promote the dissemination of knowledge in the field of crystallography to the general public of all ages and schools. This will be done through the organization of national conferences, workshops and many other events. In the near future, SCA plans to use the $CRM^2$ remote measurements platform with the support of the IUCr Africa Initiative and the African Crystallographic Association, for teaching and research activities at UASZ and UCAD.







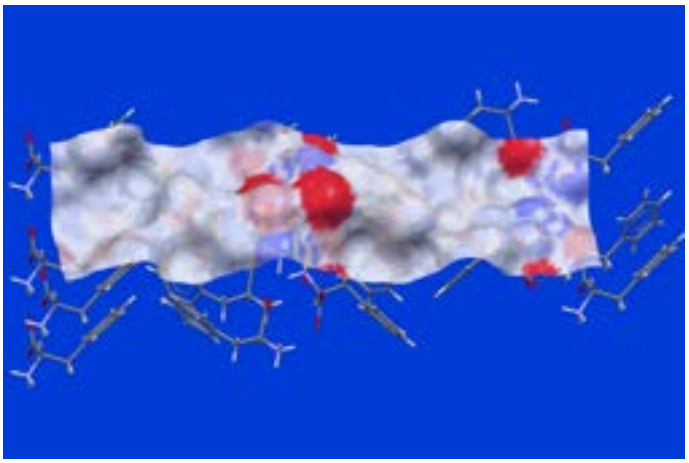




Ibrahima El Hadji Thiam is at UCAD, Senegal; Patrice Kenfack Tsobnang is at the University of Dschang, Cameroon; and Magatte Camara is at UASZ, Senegal.

SPECIAL REPORT

# News from the Cambridge Structural Database



An analysis in *CSD-Particle*: the charge on the surface of a particle is visualized. Shown on CSD Refcode QQQAUJ03 (Mossou *et al.*, 2014).

## A paper mill in crystallography — CCDC's response

In April, a pre-print article alleging a paper mill in crystallography was published. On 28 April, we at CCDC became aware of the pre-print, made a public statement on Twitter to keep the community informed and began to investigate.

The pre-print alleges that various journals have published fraudulent publications, including crystal structures. We have found 992 structures in the Cambridge Structural Database (CSD) that are associated with publications named in the pre-print. Because crystal structure data are collected into curated databases with a standard format, we have been able to investigate quickly.

For now, we have marked the structures with an editorial note so that users are aware of them. We can also provide a complete list of refcodes on request (email support@ccdc.cam.ac.uk). As the CSD mirrors the published scientific literature, we continue to work with the journals that published the work in our investigation. To date, 12 of the 992 structures have been retracted because the journals retracted the associated publications.

We are following COPE (Committee on Publication Ethics) guidelines throughout our ongoing investigation. Under these guidelines, it is important to give the authors the right to reply. We also note that even if a paper is fraudulent, the crystal structure data may not be.

From our CEO Dr Juergen Harter; "*Our proactive response to the paper mill allegations further underlines the quality and integrity of the Cambridge Structural Database and the validated, curated data that scientists use on a daily basis to guide their research and discoveries. Human interaction and intervention, by real people with domain expertise, clearly have a vital role to play to ensure data quality in an increasingly automated world.*"

To keep updated on our investigation, check for updates in our website statement here, follow us on Twitter @ccdc_cambridge or register for our monthly email newsletter.

## CCDC Engagement Grants — apply for funding to produce outreach resources

Can you inspire others with your love of crystallography? Have you got an idea for a video, social media series, game, poster or activity to get people excited about the topic?

We were excited to launch our Engagement Grants programme at the recent ECM33 meeting, as part of our charitable commitment to education in the chemical sciences.

CCDC Engagement Grants cover costs for you to produce resources or activities to increase engagement in crystallography and structural science for schools or the general public.

Key facts:

Applicants must be over 18.

Activities can be in a wide variety of formats and do not need to be in English.

You do not need prior experience in creating educational or outreach resources to apply.

We encourage people from diverse backgrounds and situations to apply.

You can apply more than once for separate activity ideas.

Activities must engage or inspire those not currently involved in STEM, including children, those undecided about what to study or the general public.

Up to £2,500 per activity is available — but we aim to fund multiple impactful projects and may not be able to provide your total requested sum.

Funds can cover licensing of software, materials and props, professional services and you and your team's time.

**Applications close on 31 October 2022** at midnight UK time.

Learn more and apply on our website here.



## New software to assess mechanical and chemical properties of particles

*CSD-Particle* software was launched in July 2022 and is available to all academics with a full CSD licence at no extra cost.

Going beyond the molecule, and the solid form, to the bulk material — *CSD-Particle* lets you predict or understand the molecular cause of manufacturing issues like sticking, wettability and tabletability in solid crystalline materials.

In *CSD-Particle* you can predict particle facets, visualize surface chemistry, charge, topology and interactions, identify potential slip planes, determine H-bond dimensionality, quantify surface chemistry and topology, and more.

Learn more and watch the 2-minute preview video here.

See all the latest updates to the CSD data and software, plus register for email updates, here.

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COMMENTARY

# Learning about CSD-Particle at the ECM33 CCDC Workshop

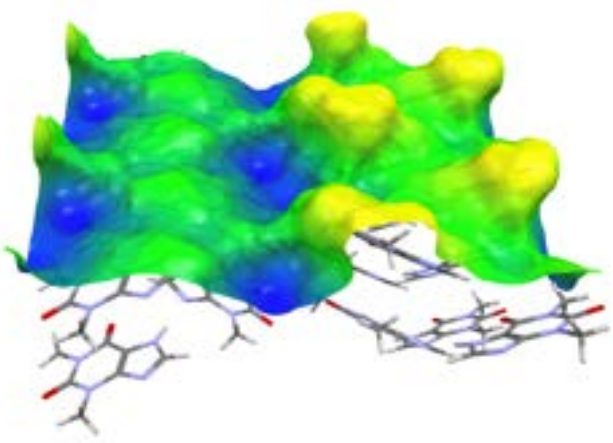


Figure 1. Visualising roughness from the topology of the (0 -1 -1) surface of theophylline form II (BAPLOT01). © CCDC.

John R. Helliwell

I arrived a day early at the 33rd European Crystallographic Meeting (ECM33) to learn how to get the most out of chemical, materials and biological structures using the latest developments made by the Cambridge Crystallographic Data Centre (CCDC) at their day-long workshop. This was in the University of Versailles, approximately a half-hour walk from the centre of Versailles. To my knowledge, this was the first time that the CCDC had included biological structures as a topic in their educational workshops. This involved learning about the biomolecular graphics program *Hermes* to accompany their chemical crystal structures program of long-standing, *Mercury*. A new product suite within *Mercury* called *CSD-Particle* was also demonstrated, enabling the rapid analysis of mechanical and chemical properties of crystalline particles. This new software tool grabbed my attention. I am not surprised it is described in news from the Cambridge Structural Database (CSD) in this issue of the *IUCr Newsletter*. My short article is not a product review (for such see *e.g.* ref [1]); rather, I describe the aspects that impressed me.

*CSD-Particle* uses computational models and algorithms, with the data from the CSD, to provide both qualitative and quantitative analyses of particle shape as well as surface and bulk properties. It provides new insights into the properties of materials. As crystallographers and structural chemists, we are very familiar with calculating, for example, the optical properties of crystals or the Mohs scale of the hardness of materials such as by Lawrence Bragg, as he describes in his book [2]. For the former, Bragg calculated the refractive indices of calcite for light travelling in the planar carbonate groups and perpendicular to them, thus quantitatively explaining the double refraction effect. For the latter, he considered the extreme examples of soft graphite or talc, with weak bonding between layers of atoms allowing the layers to slide, versus diamond with its isotropic compressibility. Also, the electrical properties of metals, semiconductors and insulators arise from the electrons in crystals arranged in so-called energy bands [3].

*CSD-Particle* offers calculations of the potential chemical interactions at a particle's surface, giving insights into its wettability, tabletability, flow and sticking potential. It also generalises the mechanical properties of a crystal by calculating its likely slip planes, related, of course, to the simple examples mentioned above. By quantification of the density of hydrogen-bond donors, acceptors, aromatic bonds, unsatisfied hydrogen-bond donors, the root mean standard deviation of the surface height, surface area, rugosity (see Fig. 1), kurtosis and skewness, *CSD-Particle* opens doors to molecular design.

I wonder if these could be applied to protein–ligand, surface to surface, interactions and the challenge of binding energy estimations [see 4]. For the latter, as emphasised by [4], the extension of static crystal structures to include molecular dynamics was necessary for a better quantitative calculation of a protein saccharide binding energy. To add experimentally determined hydrogen-atom positions using modern neutron protein crystallography would be an improvement on the X-ray only crystal structures used in [4].

The name ‘particle’ to me doesn’t quite fit the bill. As a trained physicist, it is a word reserved for ‘waves and particles’ and the ‘constituents of the atom’. To an environmentalist, its polluting particles are maybe closer to the CSD’s particle definition. In a lateral thought, and experiencing tea made in France at a café close to the ECM33 Congress Centre, I reflected on the optimum size of tea leaves. If too large, the poor surface area to volume ratio leads to too lengthy a time being needed to brew, and one’s impatience means a cup that is basically hot water and milk. For sure, though, the relationship of size, morphology, surface chemistry and function are closely related.

All in all, this new product, *CSD-Particle*, opens numerous new applied research directions in the whole topic of structure and function.

## Acknowledgements

I am very grateful to the CSD staff who hosted the training event at ECM33, namely Ilaria Gimondi, Suzanna Ward and Natalie Johnson, as well as Arie van der Lee and the local organising team, who were a great help in organising the workshop. They all did an excellent job.

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John R. Helliwell is Emeritus Professor of Chemistry at the University of Manchester, UK.

MEETING REPORT (IUCR SUPPORTED)

# Tunisian Powder Diffraction School 2022




The Tunisian Powder Diffraction School 2022 (TPDS 2022) was held at the Palais des Sciences, Monastir, Tunisia, from 27 to 30 March 2022, and organised by Drs Marwène Oumezzine and Hassen Agougui (both at Laboratoire de Physico-chimie des Matériaux, Faculté des Sciences de Monastir, Tunisia).

Powder diffraction methods have demonstrated an ever-increasing range of applications in materials science, chemistry, physics, life sciences and engineering. The purpose of the TPDS 2022 was to explore during three days the basic theory behind powder diffraction with the help and guidance of recognised experts in the field. The participants were already familiar with both the fundamentals of crystallography and X-ray powder diffraction.

This School aimed to cover all stages of sample analysis, beginning at sample preparation, experimental setup through to wavelength refinement and qualitative and quantitative analysis. In support of this, the topics covered included the following:

Basic principles of crystallography

Powder diffraction instrumentation

Physics of diffraction and crystallography in reciprocal space

Introduction to powder diffraction theory and interpretation of XRPD patterns

Powder diffraction and practical applications

and the speakers were as follows:

Professor Mohamed Oumezzine (Tunisia)

Professor Sadok Zemni (Tunisia)

Dr Rim Benali-Cherif (Algeria)

Professor Aurelian Catalin Galca (Romania)

Professor El-Eulmi Bendeif (France)

Dr Nejeb Ihzaz (Tunisia)

Dr Marwène Oumezzine (Tunisia)

Dr Ilaria Gimondi and Suzanna Ward (CCDC)

Martin Fark and Dr Tom Faske (STOE)





An Introduction to Crystallography on the first day was followed by a group discussion between the tutors and students and an oral session. The programme on the following days included practical work, lectures, further oral sessions, a poster session, a workshop on depositing and exploring data in the Cambridge Structural Database, and a presentation about STOE's powder and single-crystal XRD product range and recent installations.




Oral presentations from attendees. Left to right: Yosra Zidi (Gafsa), Chadha Mejri (Bizerte), Wael Albouchi (Bizerte) and Manel Ben Salah (Tunis).

A total of 19 young scientists (13 female, 6 male) from Morocco and Tunisia were awarded IUCr bursaries to help with travel and subsistence costs.

MEETING REPORT (IUCR SUPPORTED)

# 56th Course of the International School of Crystallography: Crystallography under extreme conditions



Annalisa Guerri

## Organization

The 56th Course of the International School of Crystallography on the subject of "Crystallography under extreme conditions: the future is bright and very compressed" was held in Erice, Italy, from 3 to 11 June 2022. The scientific organizing team consisted of Helen Maynard-Casely [Australian Nuclear Science and Technology Organization (ANSTO), Sydney, Australia], Kamil F. Dziubek [European Laboratory for Non-Linear Spectroscopy (LENS), Florence, Italy] and Shanti Deemyad (University of Utah, Salt Lake City, UT, USA). The local organizing team (the “orange scarves”) was led by Annalisa Guerri (University of Florence, Italy) and Paola Spadon (University of Padova, Italy).

## Justification

Subjecting matter to extreme conditions reveals a multitude of fascinating phenomena and is applicable to a wide range of disciplines. From the extremophiles that exist in the deepest depths of our oceans to the exotic new materials that are made when atoms are pushed ever closer together, understanding the structure of materials at extreme conditions affects biology, chemistry, physics, geoscience and material sciences. In order to achieve its goals, high-pressure research has always been at the vanguard of technical progress. It is a discipline in which equipment plays a particularly important role.

Therefore, the course covered broad ground in the application of extreme conditions crystallography. The topics ranged from fundamentals of high-pressure single-crystal and powder diffraction, through presenting the many flavors of static and dynamic compression, to reviews of sources for extreme conditions work (synchrotrons, neutrons and free-electron lasers). Complementary experimental (Mössbauer spectroscopy, X-ray magnetic circular dichroism, X-ray absorption spectroscopy, inelastic scattering) and computational methods were also discussed. Diffraction analysis on the structure of liquids, glasses and nanocrystalline materials as well as multigrain crystallography were also introduced. The lectures were harmonized with the related sessions of interactive tutorials, providing hands-on experience to the attendees. These workshops were focused on basic laboratory skills and the elements of data-processing software related to high pressure.

## Program

The school consisted of a combination of lectures and hands-on workshops, split between mornings and afternoons, respectively. The school was concurrent with the Diffuse scattering school (57th Erice Course) with three lectures shared between the two. The program consisted of 30 lectures given by 24 speakers and 3 'industry talks' provided by the sponsoring companies. Only a limited number of speakers participated remotely, with the majority of them enjoying the on-site course in the Ettore Majorana Centre. In addition, the social events and poster sessions were all shared between the two programs.

With the exception of the first day of the program, during which the lectures for the High-pressure school were held in San Rocco, all the lectures were conducted in the San Domenico facility in two morning sessions. Three hours of workshops were held each afternoon. The state-of-the art computational tools represented in the workshops included *CrysAlisPro* (single-crystal diffraction analysis), *Dioptas* and *GSAS*-II (powder data analysis), *GULP* and *XtalOpt* (crystal-structure prediction), *Igor Pro* (equation of state), *ConQuest* and *Mercury* (CCDC workshop) and *Quantum Espresso* (DFT simulations). Workshop presenters delivered tutorial instructions, data files and software downloads to participants in advance of the school. Both introductory and advanced tutorial exercises were provided in order to fully engage beginners and experts alike. In addition, hands-on workshops with detailed tutorials on diamond anvil cell loading and transport measurements were held. Three hours of lectures were presented each morning in the large (200 seat) Dirac lecture hall. Topics included a broad range of topics in high-pressure crystallography both basics and applications. These included lectures on phase transitions, crystallization, principles of powder and single-crystal diffractions, equation of state of materials, inelastic scattering, neutron scattering, high-pressure multigrain crystallography, crystal-structure predictions, complementary X-ray spectroscopy (XAS and XAFS), high-pressure microbiology, pharmaceuticals, planetary science and minerals, high magnetic fields, X-ray magnetic circular dichroism, Mössbauer spectroscopy, topological materials and communications in science. The presenters, in addition to contributing a lecture, also provided lecture notes in manuscript form. Lecture slides were also optionally made available by many of the presenters.

## Participation

In compliance with IUCr policies, the school was advertised internationally and without any geographical restrictions. Due to unusual circumstances brought about by the COVID-19 pandemic and regional conflicts, however, several of the participants could not be physically present and some of the presentations were delivered virtually. Also due to the uncertainties stemming from these conditions we had more representation from European countries. Despite these difficulties, the course successfully hosted 60 students selected out of almost 90 applications received. Sixty percent of the students and 48% of the speakers were female. It should be noted that although most of the participants were from Europe, North America and Asia, the school also accommodated scientists representing South America, Australia and Asia. IUCr funds were used to support the attendance of eight young scientists from Australia, Croatia, Israel, Portugal, Spain, Turkey, UK and USA.

## Contribution of the participants

Forty two students presented their posters at two poster sessions. The quality of the presentations was very high, in fact most of the time people were queuing up to see the displayed results. The jury consisting of the distinguished speakers representing various disciplines of extreme conditions research decided to award four poster prizes, which went to Adrien Descamps (SLAC National Accelerator Laboratory, Menlo Park, CA, USA), Viktoriia Drushliak (Adam Mickiewicz University, Poznań, Poland), Laura Henry (CEA DAM, France) and Samuel Gallego-Parra (Universitat Politècnicade València, Spain).




Winners of the poster prizes with the Directors of the course. From left to right: Kamil Dziubek, Helen Maynard-Casely, Laura Henry, Adrien Descamps, Viktoriia Drushliak, Samuel Gallego-Parra and Shanti Deemyad.

## The social program

Despite the restrictions imposed by the pandemic, the meeting organizers took every effort to facilitate the interactions between all participants. The social program was organized to take place in open areas. Conference dinner, pizza and pasta parties followed by the poster sessions, coffee breaks in an open hall, lunch and dinners in local restaurants, evening with local musicians and performers, excursions with options of guided tour to historical sites or a day at the beach followed by a banquet party, evening gatherings with local sweets and drinks and a finale dance party were all included in the program to maximize the quality time among participants. The organizers were actively participating in all the events to encourage participants to engage in conversations and create opportunities for fruitful discussions. Many students expressed that the unique dynamic atmosphere of the conference helped them build professional friendships and learn about the opportunities within the field outside of the coursework.

## Outcome

According to a survey sent to all the participants at the end of the course, the course was well received (88/100) and most of the respondents agreed that a similar school should be organized within the next 3–4 years.

MEETING REPORT (IUCR SUPPORTED)

# 10th Zürich School of Crystallography: Bring Your Own Crystals



Sepideh Rahimi (left) and Amirhossein Hajizadeh, both PhD students at the University of Antwerp, Belgium, proudly display their attendance certificates.

Hans-Beat Bürgi, Tony Linden, School Directors

The 10th Zürich School of Crystallography (19–30 June 2022) was held as usual in the Department of Chemistry at the University of Zürich (UZH), Switzerland. The 20 participants (11 female) comprised one MSc and 17 PhD students, one postdoc and one research associate. They came from 14 countries: Belgium, Croatia, Finland, Germany, Greece, Italy, Morocco, Norway, Poland, Slovakia, Slovenia, Sweden, Switzerland and Zimbabwe.



ZSC-2022 group photo.

The central goal of the School is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination so that they can competently determine their own structures when they return to their home laboratory. The daily schedule is a blend of lectures, exercises and practical work, including the opportunity to gain experience at one of the five diffractometers we have available, which include dual-source Rigaku Oxford Diffraction Synergy and Supernova instruments as well as a Bruker Venture D8 diffractometer. As usual, we had our very popular 2:1 student–tutor ratio. Lively discussions between the participants and tutors also took place outside the formal class times.

All of the participants were very engaged and enthusiastic throughout the School. The levels of experience of the participants were varied, but all came away having learnt something new and feeling better equipped to tackle their own structure determinations. Many new friendships were forged and the group was very cohesive. On the sixth day, the going got a bit tough because of a COVID-19 outbreak; three participants and three tutors tested positive and had to isolate. This necessitated implementation of hybrid sessions so that those isolating could still follow the lectures via Zoom. For the computer-based practical work this group could form their own little school in the garden of the hotel (see group photo). We are most grateful for everybody’s untiring patience and willingness to pitch in and help with other organisational matters, such as delivering meals to those isolating in the hotel. The entire group handled the problems with a fantastic team spirit.

For teaching the concepts of symmetry, in addition to online materials, we broke into small groups and used wooden and plastic models representing all point groups. The ability to hold and tumble such models helped the participants to acquire the concepts more easily. It was also great fun watching the participants cutting their apples in the "La coupe du roi" exercise to demonstrate stereochemistry and chirality.



As an introduction to structure solution and refinement, the participants worked on several example structures of varying degrees of difficulty and with different challenges. They were designed to allow the participants to see into the black box and learn about the actual procedures going on when various buttons are clicked in the software and to interpret whether or not appropriate results are obtained. Each participant then works on the data set collected from one of their own crystalline samples. We used the *OLEX2* software once again for most of the structure refinement work. The ease of use of *OLEX2* and the extensive range of tools and graphics that it incorporates, such as those for modelling disorder, allowed us to demonstrate many aspects of structure solution and refinement in a didactically beneficial way.



We no longer have a fully equipped computer classroom readily available to us because the Department of Chemistry at UZH had moved to a new building. The participants therefore had to bring their own laptops and pre-install the software we planned to use. Mostly, this worked well, with only a couple of issues, usually related to an institution-supplied loaner laptop being locked against installation of new software.

Each day concluded with a short discussion where participants could express their feelings about their experience that day and we received some valuable feedback during these moments, allowing us to tweak some aspects of our sessions on the fly. On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge.

The farewell banquet is an emotional time for everyone after making so many new friends. Each participant received a certificate, Swiss chocolate and a copy of the IUCr/OUP book *Crystal Structure Refinement, A Crystallographer's Guide to SHELXL* by Peter Müller.



Two of the IUCr-supported students, Blessed Gudyanga (Midlands State University, Gweru, Zimbabwe) (left) and Janaki Devi Somasundaram (Comenius University in Bratislava, Slovakia), with parting gifts from the School.

The questionnaire filled in by the participants provided very positive feedback, although it was clear that many found the programme too dense and that more breaks and personal study time need to be scheduled into the programme. We are considering extending the school by at least one day in 2024, but are mindful of the fact that this adds to the accommodation costs and time commitment required of the tutors. The personal impressions of three participants are given below.

This School presented some new challenges for the organisers. The closure of the hotel next to the UZH campus meant we had to find new accommodation and evening meals at a reasonable price, which is not trivial; the hotel we chose added 30 minutes each way to the day's travel time. This contributed to some of the questionnaire remarks about needing more time in the programme. We will try to optimise this for the next School.

Although we had 39 applicants for the School, 19 of them withdrew their interest, mostly because they were unable to obtain funding for their travel and subsistence. This seems to be a common problem at the moment for similar schools, such as the European Crystallography School. Although we can distribute a few bursaries using funds kindly offered by some of our sponsors (IUCr, ECA, CCDC), we cannot usually cover the full subsistence costs, let alone travel expenses. Unfortunately, there is no student accommodation in Zurich, so we are reliant on hotels and they are not cheap in Switzerland. This limits the ability of some people to attend. For example, we had three applicants from Zimbabwe, but in the end only one very talented student could attend.

We gratefully acknowledge the generosity of the sponsors and supporters: Department of Chemistry at UZH, Swiss Society of Crystallography, CCDC, ECA, IUCr, Rigaku Oxford Diffraction, Dectris Ltd, Oxford Cryosystems, Bruker AXS, Anton Paar, Eldico Scientific, OUP, and Michael Wörle for taking many photographs, some of which are in this report.

## Reports from participants

### Mateja Pisačić (Department of Chemistry, University of Zagreb, Croatia)




What an amazing experience it was to participate in the Zürich School of Crystallography 2022! Ten days of being fully devoted to crystallography flew by in a moment, but even in that relatively short time, a lot of knowledge was gained, whilst at the same time priceless memories were made.

I started my crystallographic journey a few years ago when I enrolled in PhD studies in a group where crystallography is a crucial research component. There I got familiar with some basic concepts, which allowed me to easily solve “routine” structures. However, during the research, I encountered a variety of advanced crystallographic problems, which required a proficient understanding of underlying principles in crystallography, especially X-ray diffraction. For those reasons, the Zürich School of Crystallography seemed like a perfect choice to help me obtain valuable knowledge that would allow me to overcome crystallographic obstacles. And that hypothesis proved to be true!

I must say that the organizers of the Zürich Crystallography School, Prof. Anthony Linden and Prof. Hans-Beat Bürgi, did a splendid job! Even before the school started, we were provided with thorough travel and school information and material well in advance, thus making our trip to Zürich and preparations for the school much easier. During the whole school, they carefully listened to participants’ impressions, wishes and needs, to determine if any improvements were needed, and to make us all satisfied with the school, thus ensuring that each one of us gets the most out of it, which is really impressive. They ensured that everything went smoothly, and handled every unexpected situation promptly and effectively.

The school program was quite intense but, in my opinion, very well structured, with a good ratio of theory to practice. The first two days consisted mostly of lectures, sequentially building up from basic concepts to more advanced topics. The lectures were followed by practical sessions in groups of two or five

students per tutor. I especially liked this aspect of the school, where we had a chance to discuss and resolve specific problems in detail with our tutor and obtain a further explanation of troublesome topics concerning lectures or other subjects of interest. I was very pleased that a decent amount of time was dedicated to solving structures. Starting with several example structures, we learned to treat different kinds of problems, after which we were prepared to tackle our own structures. During that time, I learned quite a lot, not only how to solve, refine and finalize the structure, but even more importantly, how to think (critically) about every step of the process and result obtained. Our tutor showed us a whole new dimension of noticing the fine details, to which I usually would not devote as much attention as needed, and these proved to be extremely informative and useful.

Another aspect that made this school unique is that we had one whole afternoon dedicated to hands-on work on the diffractometer, again in small groups of two students per tutor. We went thoroughly through the whole procedure of collecting the X-ray diffraction data, from selecting the proper crystal to setting up the measurement, with all the tips and tricks for obtaining the best possible data for a given crystal. I found this experimental session very useful, as we got a chance to ask all the specific questions concerning our usual samples and troubleshoot problems that we frequently encounter.

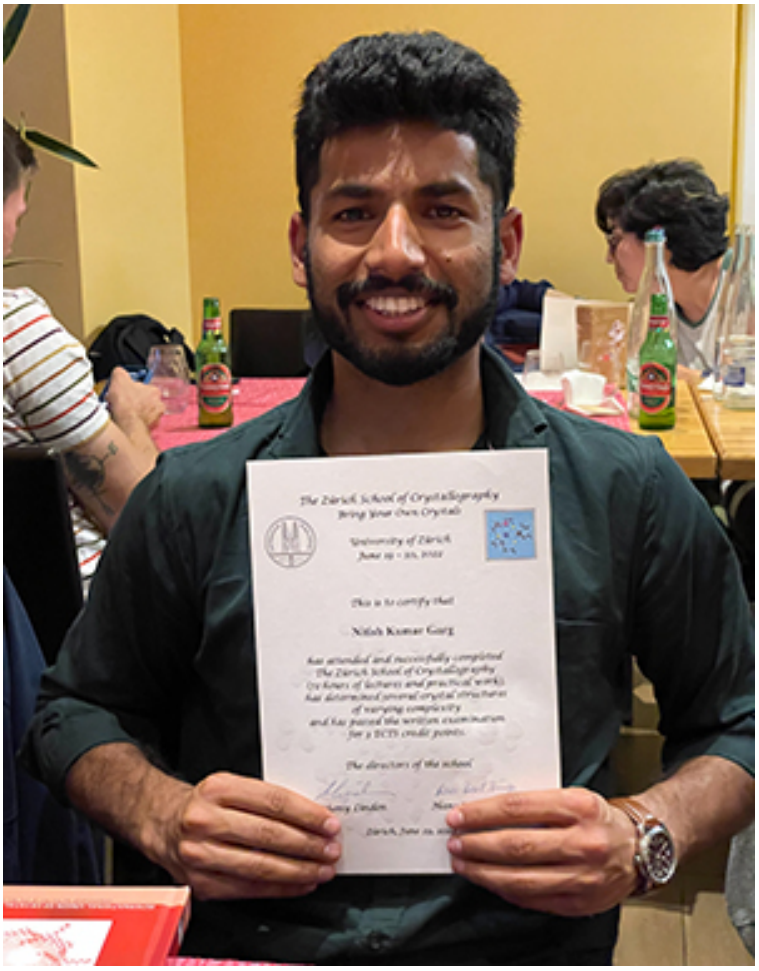
In the last day of the school, we had an opportunity to test our knowledge by taking a two-hour written exam, which I found to be quite beneficial as I got a feeling about which parts I should revise, and work harder on. I can conclude that participating in this school resolved a lot of questions I had and it provided a comprehensive overview of theory and practice in crystallography. I learned a lot of new things and reviewed some known concepts from a different perspective, which consequently shed new light on the way I will work in the future.

I must express a great gratitude and admiration to all tutors of the Zürich School of Crystallography 2022. Their unpreceded engagement in passing the knowledge to us through lectures and practical sessions, with passion and clarity, made me forget about the morning sleepiness. Instead, each day I got up motivated and excited to come to the University and explore new avenues of crystallography. Their unquestionable experience and the diversity of the scientific specialties they brought to this school allowed us to get the answers to every question asked and helped us piece together some aspects of the intricate puzzle of crystallography. I find that their devotion to providing us with answers at every conceivable moment from breakfast till bedtime, readily, patiently and relentlessly, by always finding new and creative ways to explain crystallography and challenge our knowledge in a fun and innovative way, is the true treasure of this school and its ultimate value!

And in the end, I want to express a great gratitude to Prof. Hans-Beat Bürgi and Prof. Anthony Linden for providing me with the opportunity to participate in the Zürich School of Crystallography 2022. In addition to gaining invaluable crystallographic knowledge, I met a lot of wonderful people and made new friends. All the discussions and (crystallographic and non-crystallographic) adventures we had made this school an experience I will never forget.

This school was everything I hoped for and even more! I enjoyed every single moment of it, and I would do it all over again! Thank you so much!

### Nitish Kumar Garg (Lund University, Sweden)




I recently participated in the Zürich School of Crystallography from 19 to 30 June 2022 and would like to share my experience about the school. I am a PhD student at Lund University and many of the previous PhD students from our lab, who had attended this school in past years, had recommended that I participate in this summer school. For me, who was a complete beginner in the field of crystallography, it was a wonderful opportunity to get to know about the field. I had so much to learn from the school starting from the basic theory behind diffraction of waves to finally being able to mount my own crystals on the diffractometer and further solving their structure using *OLEX2*. I felt that the course is a perfect combination of theory and practical knowledge and in such a short interval of time, the school managed to cover most of the relevant topics of the field. The fact that there is a tutor for every two students makes things easier to learn and it really helps a lot in understanding the concepts and to clear the doubts. The school had practical sessions with the tutors almost every day where we got to solve our own crystal structures and also deal with some practice structures using *OLEX2*, which helped me a lot in getting familiar with the software. I also felt that the tutors were really giving their best to make sure everyone gets the most out of the school and they were also available outside school hours for any help. Also, the course content and material given to us both before and during the course was quite helpful. I also want to mention that the school had such an excellent social environment among the students and the tutors, which is a very important part of learning and overall, I am really happy that I got the opportunity to participate in the school.

### Pawel Butkiewicz (University of Bialystok, Poland)



I became interested in crystallography during my undergraduate studies where I measured monocrystalline inorganic materials and tried to solve their structures. My knowledge, despite attending lectures on solid-state physics and studying the issues of X-ray diffraction by myself, still did not allow me to fully understand and interpret the results obtained during these experiments. I was still wondering to what extent my studies corresponded to reality and if at some point in the procedure I had not made a serious error or misconduct. As a PhD student, I found out about the Zürich School of Crystallography, and the description of the event matched what I wanted to learn. I just had to go there. I applied to the school and started fundraising. Thanks to the kindness of the director of my doctoral school, my supervisor and the ECA bursary, I secured the necessary amount.

The organizers made sure that we could fully focus on learning and talking to other participants — we were provided with accommodation and morning and evening meals, and during the breaks between lectures, we were offered coffee, tea and sweets. It is hard to imagine better learning conditions.

Step by step, we became familiar with one crystallographic question after another (starting with the question of what a crystal is, and ending with quantum crystallography) and then we performed exercises in groups of several people under the supervision and help of one of the tutors. The exercises allowed us to learn the material on an ongoing basis.

A few days after the beginning of the course, we were formed into groups of two students, and for the rest of the school, we learned to solve and refine structures together for several hours a day under the supervision of a permanent tutor.

Another element of the course, which was particularly valuable didactically, was the possibility of measuring and solving the structure of the crystal grown by hand. We were able to compare the experimental procedures and the resolution and refinement process performed by us and by the experts on the same sample, which was the best method of identifying the errors we were making.

The course ended with an exam, thanks to which we could check the extent to which we acquired the knowledge and skills passed on to us.

I learned the stages from the formation of crystals to the publication of data, I understood the concepts necessary to be a conscious crystallographer, I learned to use methods that were unknown to me, I got answers to questions that have been bothering me for years, I met wonderful people. It made my work even more interesting and gave impetus to the implementation of new research concepts. I would like to thank the organizers and lecturers of the Zürich School of Crystallography and the ECA organization as well as sponsors from my University for the opportunity to participate in the school, thanks to which I owe it all.

MEETING REPORT (IUCR SUPPORTED)

# The future of the European scientific research in crystal growth was in Paris




Matias Velazquez

From 20 to 27 July 2022, the French Committee for Crystal Growth (CFCC-French Crystallography Association) and the European Network of Crystal Growth (ENCG) co-organized in Paris, France, the third edition of the European School of Crystal Growth (ESCG3, 20–23 July) and the seventh edition of the European Conference of Crystal Growth (ECCG7, 25–27 July). These joint events were organized in association with the International Organization of Crystal Growth (IOCG) and the French Crystallography Association (AFC), and with the financial support of the IUCr. The Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung (DGKK), IUCr Journals, *CrystEngComm* (RSC) and *Crystals* (MDPI) awarded seven prizes. ECCG7 was also sponsored by AMTS and ScIDre GmbH. Additionally, AFC and the German FAIRMat initiative (FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids) hosted a booth at ECCG7.

## The ESCG3 school

Four years ago in Varna, Bulgaria (ESCG2-ECCG6), the ENCG Council had come up with several specifications for the organization of the third edition of ESCG. Firstly, the school should last four days including a Saturday to broaden its scope and save participants travel expenses between the school and the conference. Secondly, all participants should be housed at the same location for both ESCG3 and ECCG7. Thirdly, there should be discussion time between participants and lecturers. Fourthly, there should be practical demonstrations on real growth reactors and crystal pulling machines. This last demand originated from the students participating in ESCG2. While the first specification was not difficult to satisfy, the second one turned out to be a real puzzle for the organizers. In the end, only one quarter of the participants were housed at FIAP Jean Monnet, an ESCG3 venue 25-min walk from the international student center. The third specification was of course met by leaving enough time for discussion at the end of each lecture but was also satisfied by having long lunch breaks with the lecturers in the restaurants of the *Quartier Latin* district.

ESCG3 gathered 41 participants, of which 32 also attended ECCG7, and 12 lecturers (Fig. 1), mostly coming from Europe [Belgium (1), France (10), Germany (9), Italy (3), Netherlands (5), Poland (3), Romania (1), Spain (1), Switzerland (1), UK (1)] but also from Kazakhstan (1), South Korea (3), Thailand (1) and USA (1). Of the participants, 31 were either PhD students or post-doctoral researchers. Fourteen young scientists were awarded an IUCr grant to attend the school. The lectures took place in a completely refurbished and upgraded (and air-cooled) amphitheater, just the day after a heatwave had hit Paris, which meant the participants could enjoy an 8 °C temperature drop upon starting the school.



Figure 1. ESCG3 group photo, taken in front of the Curie Museum on 21 July 2022.

The international pedagogical committee worked out a broad four-day-long program (19 hours of lectures, Fig. 2), from theoretical physics of crystal growth to experimental biological crystallization, from nucleation to bulk crystal growth. All space and time scales of crystal growth phenomena were covered, in some way or another, experimentally and theoretically, not forgetting the modelling and numerical simulation approaches. Furthermore, small single crystals, bulk single crystals, eutectic composite materials, thin films and heterostructures … virtually all shapings were addressed. Cutting-edge *in situ* synchrotron X-ray radio- and topography techniques, which permit solidification interface morphological instabilities, dislocation formation and mobility, and dendrite formation to be followed ahead of the solidification interface, were also introduced. Thin-film characterizations that are closely related to their growth conditions and mechanisms were brilliantly exposed. An advanced introduction to nucleation, both classical and under microfluidic conditions, was delivered.



Figure 2. A broad review and lecture on crystal growth methods being delivered in the renovated Henri Moissan amphitheater (ENSCP-School of Chemistry of Paris).

In addition, laboratory visits and practical demonstrations on real pulling machines were organized (Figs. 3 and 4). The participants were distributed in eight groups in order to attend alternatively a total of six practical demonstrations (leading to a total amount of three hours for a given group) over three days. These practical demonstrations, on real pulling or deposition machines, including Czochralski growth, high-temperature solution growth, optical floating-zone growth, chemical vapor deposition (CVD), high-throughput membrane protein and cubic phase crystallization platforms, counterdiffusion/capillary and dialysis protein crystallization, were much appreciated by everyone, as the final roundtable discussion revealed. The commitment of the lecturers and practical demonstration chairs was total, and the participants were able to get all the lecture files, some simulation programs, many didactic videos and important textbooks at the end of the school.



Figure 3. Practical lectures on biological crystallization at the Institut of Physico-Chemical Biology (IBPC) (lecturers: Françoise Bonneté, Monika Spano and Franck Brachet).

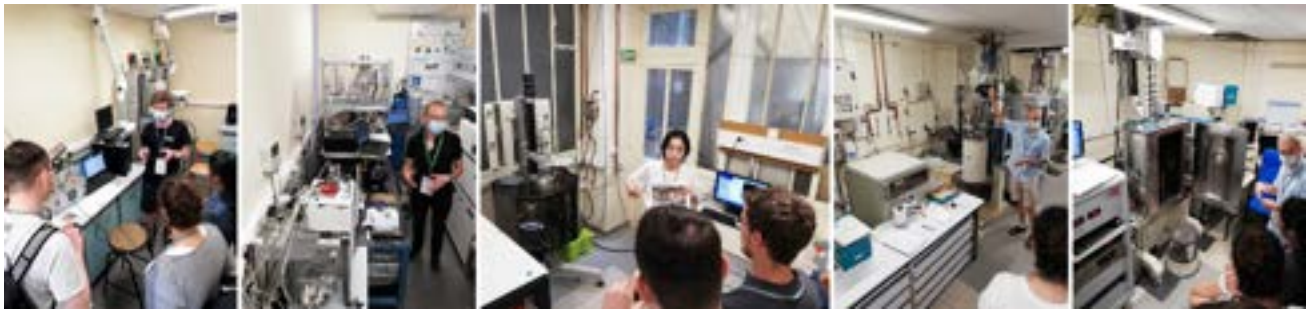


Figure 4. Practical lectures on high-temperature solution growth, thin-film growth by CVD, optical floating zone furnace and Czochralski growth at the Institut de Recherche Chimie-Paris (IRCP) (lecturers: Florent Cassouret, Alexandre Tallaire, Haichao Lan and Pascal Loiseau).

## The ECCG7 conference

For this seventh edition of ECCG, following the recommendations of the ENCG council and in synergy with both the international scientific and the program committees, the organizers had to implement a scientific program with a broader scope. Consequently, 14 sessions, 3 parallel sessions and double the number of plenary lectures were implemented. A particular effort was made to substantially increase the participation of early-career scientists in session invited lectures, oral communications and poster communications. Seven awards publicized worldwide were delivered. Moreover, the organizers publicly endorsed the IUCr GEDC Code of Conduct, which — among other things – requested that attention should be paid to gender balance and affiliation country balance in all organization and scientific aspects of the conference. Hence, a few days before the events started, the organizers published on the ESCG3–ECCG7 website detailed statistics about gender balance and affiliation country in ECCG7 international scientific and program committees composition, ESCG3 international pedagogical committee composition, ESCG3 lecturers list, ECCG7 session chairs composition, invited lectures (both plenary and session), oral communications and so on. Five of the 24 session invited lectures, as well as 32 of the 77 oral communications and 57% of the poster presentations were delivered by early-career scientists. Seventeen young scientists were awarded an IUCr grant to attend the conference, among which 13 had attended the school too (Fig. 5). Of the 17 IUCr grant awardees, 10 were women, and if we add ECCG6 and ECCG7 best poster and best oral communication awards, a total number of 5 women awarded over 11 prizes is reached.



Figure 5. ECCG7 IUCr grant awardees photo, taken during the award ceremony in the main conference room on 27 July 2022.

During the ECCG7 welcome address, Andrea Zappettini, the active ENCG coordinator, made an ENCG statement to condemn the war in Ukraine, and express ENCG solidarity with colleagues from the countries involved in the war and suffering from its consequences.

The ECCG7 gathered 223 participants (Fig. 6) from 34 countries around the world but with a main (quantitative) contribution from France, Germany, Poland, UK, Italy, the Netherlands and Switzerland.



Figure 6. ECCG7 group photo, taken in the main conference room on 26 July 2022.

A total of 206 abstracts were submitted from 32 countries around the world with main (quantitative) contributions from France, Germany, Poland, Italy, USA, the Netherlands, Switzerland and UK. The most popular sessions in terms of abstract submissions were Fundamentals of Nucleation and Crystal Growth & Digitization in Crystal Growth; Surfaces, Interfaces, Epitaxial Growth & Growth at the Nanoscale (dedicated to the memory of Ivan V. Markov 1941–2022); Semiconductors; Optical Crystals; and

Functional Crystals. The smaller Mineral Growth Processes session proved to be particularly vivid and outstanding, and the Crystallization of Organic Materials & Industrial Crystallization Process Engineering and Crystallization of Biological Molecules and/or in Biological Systems sessions also attracted a significant audience for the first time during an ECCG event. The program contained four invited plenary lectures, which were chosen according to the topical coverage of the conference, gender balance and affiliation country. All of them were absolutely brilliant and triggered interesting discussions. The first one, entitled Step-growth, impurities and mass transport: the surprising complexities revealed by simulation, introduced the full session on Fundamentals of Nucleation and Crystal Growth, and was delivered by James F. Lutsko (Université Libre de Bruxelles, Belgium). The second one, entitled Can the crystal structures of pharmaceuticals be predicted?, closely related to the session on Crystallization of Organic Materials & Industrial Crystallization Process Engineering, was delivered by Sarah (Sally) L. Price (FRS) (University College London, UK). The third one, entitled Recent advances in protein crystal growth, introduced the session on Crystallization of Biological Molecules and/or in Biological Systems, and was delivered by Simona Fermani (University of Bologna, Italy). The fourth one, entitled The physical chemistry of oxide molecular beam epitaxy, introduced the session on Surfaces, Interfaces, Epitaxial Growth, Thin Films & Growth at the Nanoscale, and was delivered by Oliver Bierwagen (Paul Drude Institute for Solid State Electronics, Berlin, Germany). In addition to these, 24 invited session lectures, 77 oral communications and 92 poster presentations distributed among the 14 session topics were delivered.

On 26 July, the participants enjoyed a gala dinner on the Seine riverboat Le Jean-Bruel. The weather and temperature were just perfect for a nice summer evening cruising past most of the well-known Paris monuments.

The following prizes were awarded (see Fig. 7).

Prize

Recipient

Contribution

Presenter

DGKK best (ESCG3) student ECCG7 poster prize

Martina Cotti (Eindhoven University of Technology, the Netherlands)

Understanding the link in between hydration kinetics of $CuSO_4$ powder and mm-tablets

Andreas Danilewsky

*Acta Cryst. B* Crystal growth section best oral communication awards for early-career scientists

Marloes Bisterwels (AMOLF, Amsterdam, the Netherlands)

Light-controlled nucleation and shaping of self-assembling nanocomposites

Geetha Balakrishnan, Chair, IUCr Commission on Crystal Growth and Characterization of Materials

Adrienn Maria Szucs (Trinity College Dublin, Ireland)

Crystallization pathways towards bastnäsite: the role of dolomite and aragonite in the formation of rare earth carbonates

*CrystEngComm* best poster award

Ondřej Černohorský (Institute of Photonics and Electronics, Czech Academy of Sciences, Prague, Czech Republic)

Chemical calculations in modelling of low-temperature growth of ZnO nanowires

Andrea Zappettini

*CrystEngComm* best oral communication award

Yvonne Tomm (Helmholtz-Zentrum Berlin für Materialien und Energie, Germany)

The same but different: Single Crystals of Quaternary Adamantines by Chemical Vapor Transport

Andrea Zappettini

*Crystals* best oral communication prize for an early-career scientist

Merve Kabukcuoğlu [Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany]

Evolution of Dislocations in GaAs Wafers under Processing relevant Conditions Studied by 2D and 3D X-ray Diffraction Imaging

Andrea Zappettini

*Crystals* best oral communication prize for a senior scientist

Frédéric Leroy (Aix-Marseille Université, France)

Ferroelectric nanodomains in epitaxial GeTe thin films

Andrea Zappettini



Figure 7. ECCG7 award ceremony. From left to right: Andreas Danilewsky delivered the DGKK prize to Martina Cotti, Geetha Balakrishnan delivered the *Acta Cryst. B* Crystal growth section prizes to Marloes Bisterwels and Adrienn Maria Szucs, and Andrea Zappettini delivered the *CrystEngComm* and *Crystals* prizes to Ondřej Černohorský and Merve Kabukcuoğlu.

Finally, the ENCG Council met on 26 July and decided that the 4th ESCG and 8th ECCG events would be organized in Warsaw, Poland, in June or July 2024. It also elected its new Executive Committee: Thomas Schröder (Germany, ENCG coordinator), Linda Pastero (Italy, scientific secretary), Mike Leszczynski (Poland, ECCG8 chair) and Matias Velazquez (France, ECCG7 chair). The whole Council thanked Andrea Zappettini, Florinda Costa and Bogdan Ranguelov for serving on the Executive Committee, and Daniel Vizman for his support as ENCG webmaster.

MEETING REPORT (IUCR SUPPORTED)

# 72nd Annual Meeting of the American Crystallographic Association (ACA2022)




Brandon Q. Mercado

The 72nd Annual Meeting of the American Crystallographic Association was held in Portland, OR, USA. The scientific program spanned 30 July–3 August 2022, with associated workshops on 29 July. The program consisted of 40 scientific sessions, 2 evening sessions, 3 poster sessions, 8 workshops and a 3-minute thesis competition. This meeting hosted several firsts for attendees, including an art exhibit with 24 contributions viewable at the final poster session and awards banquet. All attendees wore masks and enjoyed a safe return to interacting with booth hosts in the exhibition hall. Thanks to the remarkable work of many volunteers and organizers, ACA2022 was able to offer all sessions as in-person, with some in-person and live-broadcast sessions with virtual participation. The meeting was well-attended, with over 500 registrants and over 200 workshop participants.

We are extremely proud and happy to relay that only four cases of COVID were reported during the meeting. According to our policy, those individuals did not return to the meeting space, and all close contacts were immediately notified. We received three reports of mild COVID cases in the 14 days following the meeting. This meeting was able to safely take place in-person thanks to the conscientious participation of everyone involved in wearing masks, sanitizing hands and respecting social distancing boundaries. Thank you to all meeting participants for helping to exceed our safety expectations!

The scientific program opened with a keynote address from David Baker, whose lecture was as engaging as it was wide-ranging. He spoke on the use of *RoseTTAFold* and related software to predict COVID binding molecules, targeted delivery with plug-proteins, designer molecular machines and many other topics. A panel of six researchers responsible for Professor Baker's various projects fielded many questions from the attendees (Fig. 1). The following day opened with five simultaneous sessions. The two hybrid sessions focused on timely and highly publicized topics: COVID and Artificial Intelligence/Deep Learning. The Transactions Symposium, "The Role of Structural Science in Tackling a Pandemic: COVID-19 as a Paradigm," expounded on many lessons we learned about COVID-19 and pandemics over the past two years. Next door, "Use of AI predicted Models in Structural Biology/Crystallography" expanded on many topics featured in the keynote. Minkyung Baek spoke more on the utilities of *RoseTTAFold*, while Thomas Terwilliger and Jennifer Madrigal dissected the details of *AlphaFold*. The subsequent three days continued with parallel scientific sessions and poster sessions.



Figure 1. Question and answer session during David Baker's keynote address at the welcome reception.

Another highlight of the meeting was the "What I Learned from my 1st Structures" session, in which presenters worked chronologically from youngest to oldest in sharing their early experiences. The session started with Shbham Dubey (Purdue), who gave a fabulous talk about her current graduate school adventures in working through her first structures of the Tpb system of pathogenic *Neisseria*. The more experienced presenters in the session mixed fun stories of their earliest crystallography experiences and how these experiences provided life lessons that impacted their personal and professional growth.

This year's program truly embraced our new logo and name, ACA: The Structural Science Society. We saw more talks covering structural techniques outside of traditional crystallography, such as Flora Meilleur's (Oak Ridge National Lab) talk about neutron diffraction in the "Hot Structures" session. We also saw more sessions covering various cryoEM methods, such as the "New Developments in cryoEM and cryoET: Towards Atomic Resolution" session, as well as the "MicroED of small and macromolecules" session (Fig. 2).



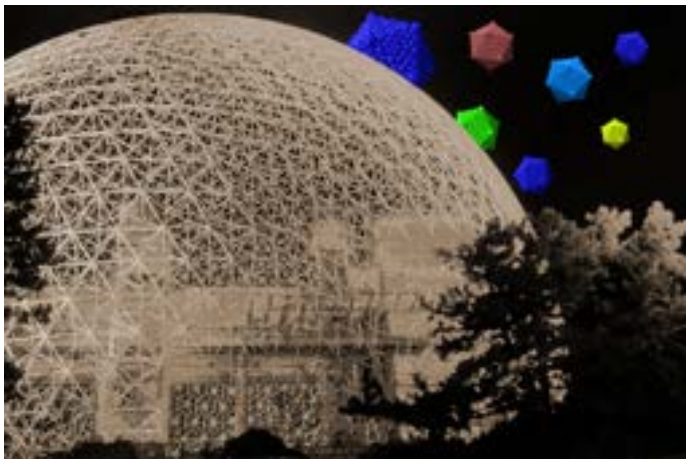
Figure 2. Speakers and organizers of the session "MicroED of small and macromolecules." Left to right: Anna Shiriaeva, Emma Danelius, Jungyoun Cho, Joseph Ferrara, Tamir Gonen, Jessica Bruhn, Anchi Cheng and Abhay Kotecha.

Details on this and future meetings can be found at www.acameeting.com. More information can be found at our social media accounts on Twitter and Instagram @ACAxtal, Facebook @AmerCrystalAssn or LinkedIn. In anticipation of an in-person meeting for 2023, please mark your calendars to join us 7–12 July in Baltimore, MD!

The ACA2022 Abstracts are available in a special supplement to Acta Cryst. A.

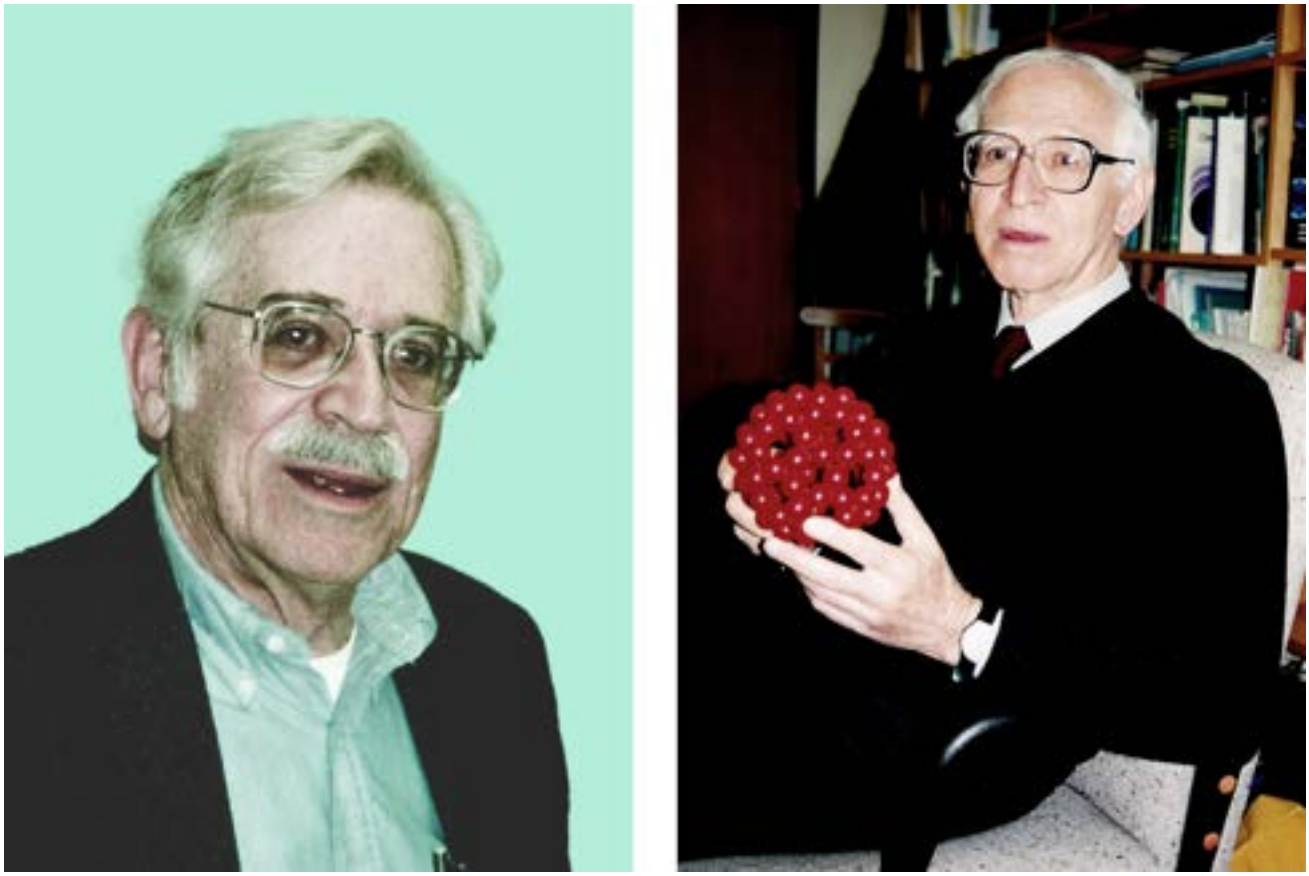
HISTORY OF CRYSTALLOGRAPHY

# Viruses and geodesic domes – Donald Caspar, Aaron Klug and Buckminster Fuller



Istvan Hargittai, Magdolna Hargittai

Donald L. D. Caspar (1928–2021), a pioneer in understanding virus structures, passed away recently [1]. In this note, we talk about his cooperation with Aaron Klug (1926–2018). We also mention the influence of the geodesic dome, designed by R. Buckminster Fuller (1895–1983), on the research of virus structures. In conclusion, we quote excerpts from our 1996 conversation with Caspar.



Left: Donald L. D. Caspar (1996) in Tallahassee, FL, USA. Right: Aaron Klug with a spherical model (2000) in Cambridge, UK. Both photographs by the Hargittais.

Caspar was born in Ithaca, NY, USA. Already at the age of 10, he became acquainted with interesting science. Through his chemistry graduate student father, he met the renowned crystallographer Isidor

Fankuchen, who told him about the tobacco mosaic virus (TMV). Caspar studied at Cornell University (BA in physics, 1950) and at Yale University (PhD in biophysics, 1955). His dissertation was on the radial structure of TMV. At Yale, the research was focused on radiation biology, and biological structures were investigated by destroying them with X-rays, protons and deuterons. However, he thought that using X-ray scattering may be more instructive, and he carried out small-angle X-ray diffraction on TMV. He produced the second isomorphous derivative of a biological structure after the isomorphous derivative of hemoglobin by Max Perutz [2].

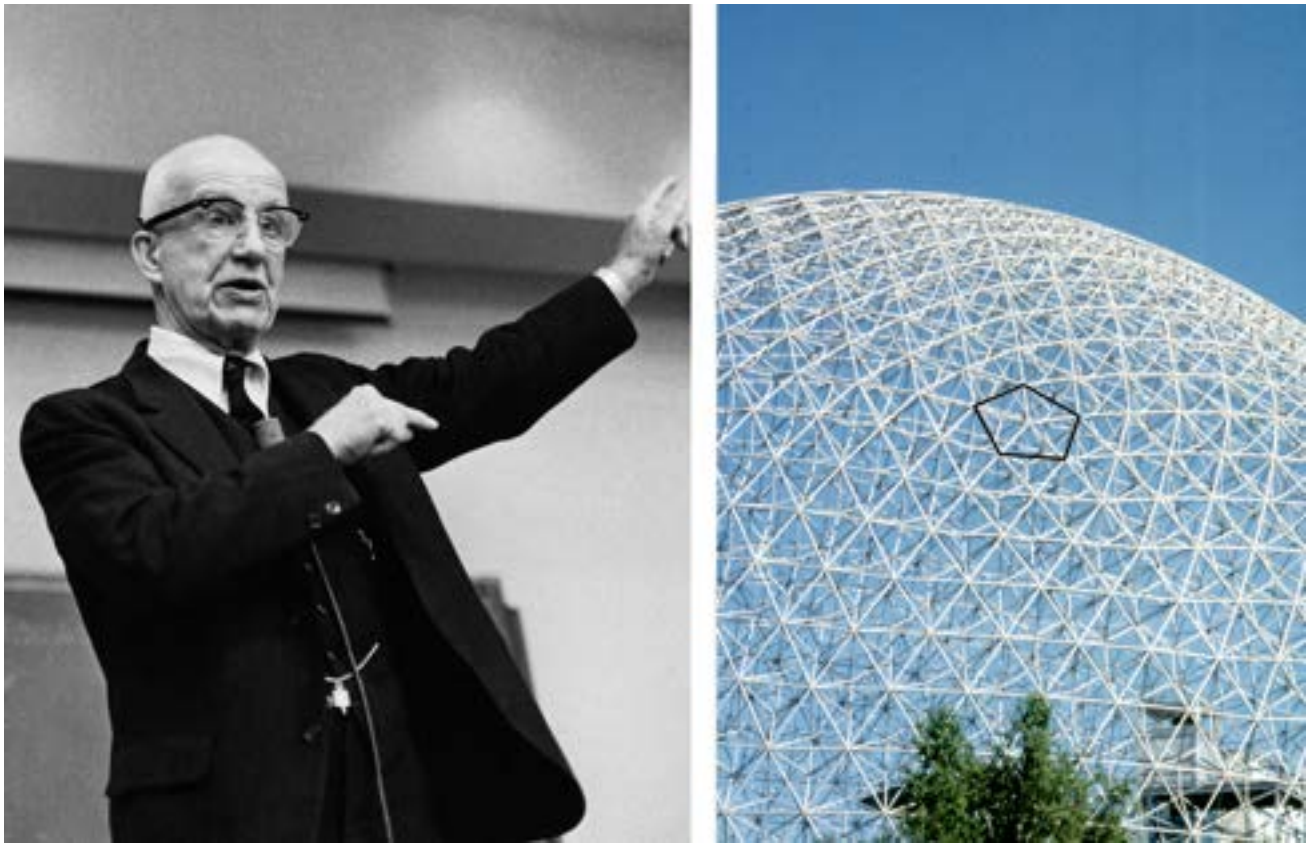
In 1954, Caspar moved to the California Institute of Technology (Caltech). Formally, he was in Max Delbrück's laboratory but was involved mostly in X-ray crystallography with Linus Pauling. Caspar used to build models of nucleic acids and viruses with James D. Watson. Eventually, he joined the Children's Cancer Foundation at Harvard Medical School, where he built models of icosahedral viruses. He went to Cambridge, UK, in 1955.

It was about this time that Aaron Klug met Buckminster Fuller, who visited Birkbeck College of London University. Klug was also interested in virus structures and recognized that there was some relationship between Fuller's work on geodesic domes and virus structures. Klug was born in Lithuania, and his family moved to South Africa when he was two years old. He studied at the University of Witwatersrand in Johannesburg and at the University of Cape Town. He continued in Cambridge and earned his doctorate in 1952. He was at Birkbeck College between 1954 and 1961, and at the Medical Research Council (MRC) Laboratory of Molecular Biology from 1962 for the rest of his career. He was one of the most distinguished British scientists. He received the Nobel Prize in Chemistry in 1982 for electron crystallography and the determination of complex nucleic acid–protein biological structures. He received the Copley Medal of the Royal Society in 1985, was a member of the Order of Merit and President of the Royal Society (1996–2000).

Fuller made constructions from early childhood throughout his long life. He enrolled at Harvard University, but was a maverick and a rebel and never graduated. His main work was his two-volume *Synergetics* [3], in which he followed Aristotle's maxim, "The whole is more than the sum of parts." Fuller built his first geodesic dome in 1947; it was a re-invention because such domes had been built before, but his constructions became famous. In the wake of his activities, many companies built a large number of geodesic domes over the years. *Synergetics* contains many interesting ideas, and many of them appear to have been taken from others, but Fuller was known not to indicate sources or references and not to acknowledge the contributions of others. But he impacted the research directions even of genuine scientists, such as Caspar and Klug.

Klug chose to investigate spherical viruses when developing his own research project at Birkbeck College. There was a tradition of such studies at Birkbeck. J. Desmond Bernal and Harry Carlisle took the first X-ray pictures of spherical virus crystals in the late 1930s. Rosalind Franklin made important advances by solving the structure of the protein helix of the virus, without the RNA. When Caspar joined Birkbeck College, he and Klug teamed up and found crystals of viruses in the refrigerator [4, p. 315]. Caspar took the bushy stunt virus and Klug the turnip yellow mosaic virus.

In 1962, Caspar and Klug published their discovery of the icosahedral virus structures in a seminal paper [5]. They profusely thanked Fuller for the inspiration they received from his creations, and one of their illustrations was a Fuller geodesic dome. They noted that the resemblance of the geodesic domes to the virus structures attracted their attention. By the time Fuller visited Birkbeck, Caspar had returned to the United States, but Klug attended Fuller's presentations. They were not easy to absorb because Fuller spoke a peculiar language. Klug noted about one of Fuller's books that he was interested in reading, but he had to 'translate' Fuller's peculiar English into an English understood by everybody else. Klug referred to Fuller as "a Yankee inventor, practical, totally untheoretical" [4, p. 316].



Left: R. Buckminster Fuller (1970) at Pacific High School, Saratoga, CA. Photograph by and courtesy of Lloyd Kahn. Reproduced with permission. Right: Section of Fuller's geodesic dome built for the 1967 Montreal Expo. Photograph by the Hargittais. One of the pentagons among the hexagons is highlighted.

Caspar and Klug introduced quasi-equivalence among the large number of identical protein subunits of the virus structure, and this light deviation, however, from perfect symmetry, raised eyebrows. In hindsight, we may consider this as a forerunner of what quasicrystals represent, certainly an extension of classical crystallography. When Caspar and Klug initially proposed quasi-equivalence in their description of virus structures, Klug remembered "Max Perutz said in an interview in *Science* in 1966 that Klug was telling us these 'most unlikely stories'" [4, pp. 316–317]. According to Klug, Perutz thought that the protein units could not adapt to their environments because they were rigid. Caspar and Klug built their ideas on the notion that proteins had flexibility. They stressed that the chemical structures did not have to satisfy the requirements of exact mathematical principles; instead, they had to *satisfy the requirement of reaching a minimum energy configuration.*

Caspar had two major appointments consecutively. Between 1972 and 1994, he was Professor of Physics and Research Professor of Structural Biology at the Rosenstiel Basic Medical Sciences Research Center, Brandeis University. He has been credited with coining the expression "structural biology". Then, he was Professor of Biology at the Institute of Molecular Biophysics, Florida State University in Tallahassee. It was there that we visited him in 1996 and recorded a long conversation with him. His activities crossed disciplinary lines between physics, chemistry and biology, and involved viruses, fullerenes and quasicrystals. We quote a few excerpts from our conversation [6]:

On fullerenes:

"*Our theory for icosahedral virus design accounts well for the design of fullerenes. The basic geometry of hexamers and pentamers forming closed shells leads to icosahedral symmetry, which is the most regular way to do this.*"

On quasicrystals:

"*Quasicrystals are more interesting than crystals in the traditional sense. In the quasicrystal the same atom may take different positions with equal probability. But even in a quasicrystal one can categorize*

*the atomic motifs and their number is limited. These motifs with local pentagonal or icosahedral symmetry can be combined in many different ways to generate quasi-periodic lattices. The activation energy of switching from one arrangement to another though is probably very high. However, in the growth process, the different arrangements are of equal probability. Thus there is no way of predicting which way the atom is going to go when the atoms are assembling.*"

On the general versus the individual:

"*In physics, the greatest concern is in finding the underlying, unifying principle: abstracting out all the individuality, the differences among all sorts of systems to come down to some basic core. When I started in biology, I had a feeling that the use of such an approach would be constructive in understanding biological organization. Today, I think it is only a crude first step. Maybe we do find some generalization that is helpful for our comparing and categorizing of different systems, for example, the structural organization of different viruses. Almost all isomeric virus particles have icosahedral symmetry. But when we come down to such a core, we realize that what appears interesting in biology is not the underlying principle but the individual properties. … The uniqueness of the individual may not exemplify the properties of the group. There is some paradox here, and this makes biology so fascinating.*"

## Literature

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[6] Hargittai, I. & Hargittai, M. Unpublished conversation with Donald L. D. Caspar, 28 November 1996, at the Institute of Molecular Biophysics, Florida State University, Tallahassee. Other excerpts from this conversation have appeared in Hargittai, I. & Hargittai, M. (2000). *In Our Own Image: Personal Symmetry in Discovery*, pp. 11, 56–57, 92–93, 96, 177. New York: Kluwer/Plenum.

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PRESS RELEASE

# Kent Heath named new CEO of Rigaku Americas Holding Inc. and President of Rigaku Americas Corporation



Rigaku Americas Holding Inc., the North American subsidiary of Rigaku Corporation, Japan's leading manufacturer of X-ray analysis, measurement and testing instruments, has recently announced Kent Heath as its new CEO. Heath was also named President of Rigaku Americas Corporation.

Heath is the former VP and GM of the Tribology, Stylus and Optical Metrology business unit with Bruker Corporation and previously Vice President of Strategic Marketing in Bruker's Nano Group. He has more than 30 years of experience in the semiconductor, network equipment and analytical device space, including a 10-year spell with Motorola Semiconductor, where he led a turnaround of their wireless business in Japan. He has a proven track record of building strong, high-performance teams and driving commercial excellence in a wide range of industries, including test and measurement equipment, wireless networking and high-performance semiconductors.

Toshiyuki Ikeda, Group CEO at Rigaku Holdings Corporation in Japan, commented, "We are very pleased that Kent has joined us at Rigaku. We believe he will be a great asset as we build out a global team to bring our best-in-class analytical instruments to a wider market."

Heath commented, "I am very excited to be joining Rigaku. With their wealth of experience in X-ray analytical solutions, there is strong potential for further growing the business in the Americas. I am looking forward to working with the Rigaku team and helping to drive the company to the next level."

Please visit https://www.rigaku.com/ for more on Rigaku.

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