

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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LETTER FROM THE PRESIDENT

The changing meeting scene

Sven Lidin



I started to study for my PhD in 1986. Since then I have attended conferences every summer, often several, sometimes far too many. The value of maintaining close contact with old friends and research partners, in combination with meeting new people with new ideas and impulses, is considerable - without a doubt. What has been particularly valuable for me has been exposure to activities that are some way away from my own field where I am faced with unexpected approaches. I have certainly expanded my research register and all these encounters have undoubtedly made me grow, but have I used my time in the best possible way? Would it have been more productive to spend time recovering?

I have no idea, but it would be naive to believe that these 35 years of busy summers have constituted an optimal strategy.

The conference and meeting merry-go-round has stopped and when it starts turning again I hope that we have learned from the period we have been through. We can reduce impacts, both on the environment and on ourselves, if we travel a little less. Having said that, we cannot completely refrain from physical meetings - my experience from digital meetings is that some work well, whereas others present difficulties.

The [IUCr Congress and General Assembly](#) was postponed for a year, but the Executive and Finance Committees of the IUCr met according to schedule, if not according to plan. During one week in August, we found a daily time slot that was convenient for us Europeans, rather late for our friends in Japan and Australia and rather more early for our friends in the Americas. You all know the drill: in virtual meetings

you avoid the jet lag, but you pay by odd working hours. As you all know, it works. We got the work done.

Certainly, there are aspects of meetings that work excellently on *Zoom*, but not all and not all the time. Certainly, we can communicate with colleagues without always having to meet, but we are still individuals with considerable social needs. Trust and a sense of belonging are created so much faster and more strongly in real life than online. Meetings online may be excellent for exchanging information or for making decisions, but you leave online meetings a little more tired than when you went in. A physical meeting, on the other hand, may charge you with energy and enjoyment.

The crystallographic community is a friendly one and I miss my friends.

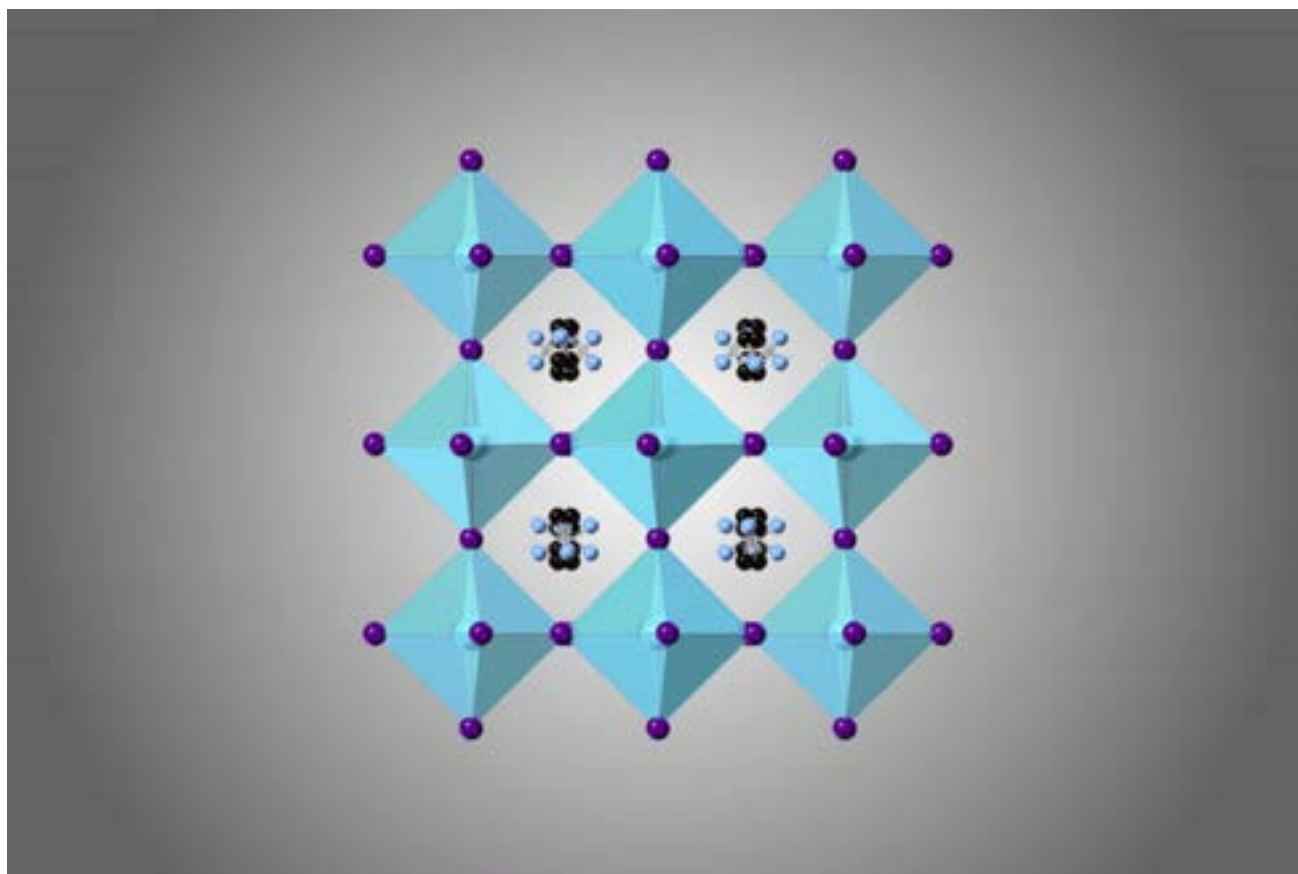
I miss you all.

A couple of weeks ago I was involved in welcoming our new incoming international students to Sweden. In meeting the group, I re-experienced the exhilarating feeling I used to have when standing in front of a new class of students. For me, the meeting - that magical meeting - is not a digital phenomenon, it requires physical presence. I look forward very much to a more open teaching and meeting environment, but until then, let's continue onwards on *Teams* and *Zoom*!

EDITORIAL

Editorial

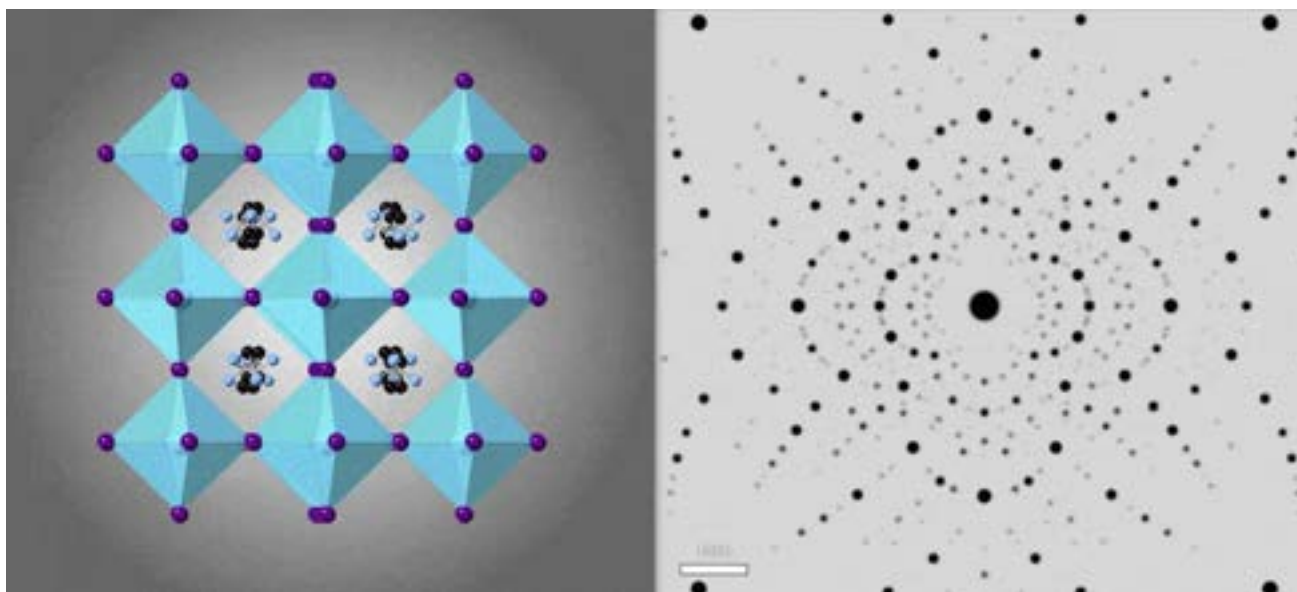
Mike Glazer



The COVID-19 crisis continues to spread throughout the world, with worryingly large outbreaks occurring. Although in many countries restrictions have eased, the recent trends are disturbing, and I think we are all in for a bumpy ride in the next few months. As we saw [in the last IUCr Newsletter](#), crystallography has been playing a significant role in helping to understand the SARS-CoV-2 virus, a vital area of research. Such research is often taking place through national facilities such as synchrotrons, neutron sources, and of course, electron microscopes. Crystallographers are well used to working with X-rays, neutrons and electrons as part of the fight against this deadly pandemic. Almost uniquely amongst all the sciences, we are exceptionally fortunate to have our own scientific union, the International Union of Crystallography (IUCr), and so we crystallographers are well used to international collaboration, which is necessary to make progress in this field.

So what do we have in this issue of the *Newsletter*? Science is full of forgotten scientists who played essential roles in the development of the science we see today. I think that it is useful to look back from time to time to understand who they were. One of these is Walter Friedrich. We publish a [report](#) translated by Peter Heaney and Melanie Kaliwoda on a rare interview with Friedrich, who, in 1912, together with Paul Knipping, was the first to obtain X-ray diffraction images from crystals, thus showing that X-rays had the properties of waves. Both of them have largely been forgotten, for it was their leader Max von Laue who gained the 1914 Nobel Prize for this work. It was this work that then led W. H. and W. L. Bragg in the same year to establish a new scientific discipline: X-ray crystallography. This, after all, is the subject that is today playing such an important part in research into the SARS-CoV-2 virus. Friedrich and Knipping had to work under challenging conditions, apparently, as Laue was not able to persuade his

boss, Arnold Sommerfeld, that the experiments were worth undertaking. As an aside, I recall many years ago during an IUCr Congress that Paul Ewald, who had been a student of Sommerfeld's in 1912, told me that Friedrich and Knipping secretly "stole" Röntgen's X-ray apparatus to carry out the tests!



Another largely forgotten scientist is Jan Czochralski, whose name is well known among crystal growers in connection with the so-called Czochralski method. But who, in fact, was Czochralski? In which country did he live, and what did he do? Many think he was an American scientist of Polish origin, but this was not the case. For years his story was kept in the dark, but today in his native Poland, after years of ignominy, he is celebrated as a hero. How has this come about? It is an interesting [story](#), full of mystery and intrigue, a life set against the terrible events of the Second World War in Germany and Poland.

Recently, the Royal Mint in the UK has produced an excellent new 50 pence coin celebrating the famous Photo 51 of Rosalind Franklin. This caused some discussion on Twitter, mostly as it was not obvious what the image on the coin actually showed. You can read about this coin [here](#) and how to obtain one for yourself.

The IUCr together with UNESCO has been active for several years in promoting crystallography in Africa, and the benefits of this are becoming apparent. In this issue, we have [an article](#) written by a young crystallographer in Benin, Sidoine Bonou, who describes his own journey into research and his visits to Italy to learn the crystallographic arts. He describes his travel to Naples, Bari and Trieste in order to gain a wide experience. As he points out, significantly, it was the first time he had the opportunity to visit a synchrotron.

I was pleased to hear that the Royal Swedish Academy of Sciences has decided to award the [Gregori Aminoff Prize 2021](#) to Henry Chapman (University of Hamburg, Germany), Janos Hajdu (Uppsala University, Sweden) and John Spence (Arizona State University, Tempe, AZ, USA) "for their fundamental contributions to the development of X-ray free electron laser based structural biology". The Gregori Aminoff Prize is an international prize awarded since 1979 by the Royal Swedish Academy of Sciences in the field of crystallography.

Finally, there has been a new addition to the Royal Society *Biographical Memoirs*, which will be of interest to crystallographers. This is about Ken Jack, who worked on three main areas of materials science: metals, glasses and ceramics. See [here](#).

Stay safe!

LETTER TO THE EDITOR

Proposal for PDB deposits to include contact details for senior author

Wladek Minor | John R. Helliwell



The Chairs of the [IUCr Commission on Biological Macromolecules \(CMB\)](#) and the [IUCr Committee on Data \(CommDat\)](#) together with a number of prominent crystallographers have written the following letter to the [Worldwide Protein Data Bank \(wwPDB\)](#):

During recent years we have observed a growing number of deposits that, instead of listing a journal as the primary citation, have a “To be published” status. As of 12 June 2020 there were more than 26,000 PDB deposits that have “To be published” status and more than 9,000 deposits have held this status since 2010, i.e. for 10 years.

Core metadata are very important for biomedical scientists as well as structural biologists. However, when we are working on a similar structure we often need additional information that is impossible to obtain from the PDB deposit alone. In particular, when a PDB deposit has a journal publication as a primary citation, it is very easy to find an email address of the senior author (or depositing author) and contact that person if the need arises. Unfortunately, this is often not possible in the case when the primary citation has “To be published” as its status in the PDB.

We, the Chair of CBM, the Chair of CommDat and other senior crystallographers, propose that every PDB deposit should have in the metadata for the deposition the work institution email address of the senior author. We hope that this would allow for easy contact with the authors of

every PDB structure in case of any query. Also we think it could reduce the number of places on the internet that keep 'independently validated' versions of a structure.

Crystallographers who would like to support this initiative should send an email to CBM Chair [Wladek Minor](#) or CommDat Chair [John Helliwell](#).

IUCr ACTIVITIES

COVID-19 and the IUCr

Alex Ashcroft



It has been a while since most of the IUCr staff have seen their offices (indicated in red) in Chester, UK, but here is a reminder, courtesy of [DronePics.Wales](#), licensed under [CC BY 4.0](#).

In mid-March, I posted an announcement on the IUCr website to say that IUCr staff were following government guidelines and working from home as much as possible. Seven months on and little has changed. Thanks to the expertise and dedication of the R&D staff in keeping our systems running and the professionalism and adaptability of the editorial staff, things are largely still functioning as normal despite the prolonged absence from the offices of most members of staff. We are determined to continue to provide the levels of service that you expect from IUCr Journals, so if you are encountering any problems, please do let us know. I was delighted to be copied on the following feedback from one of our authors recently: “As usual, what we will publish is better than what I submitted. This is the normal situation when publishing in IUCr journals (in contrast to virtually all other publishers).” Apart from reporting any problems, any positive feedback is always gratefully received. A staff working group has even found the time to complete the redesign of the [IUCr website](#), culminating in a vibrant and well organised homepage whose colours are based on those of the IUCr Journals. This homepage provides easy access to all areas of the site, including *IUCr Newsletter* articles so you can stay in touch with news from the community. New minisites have been created (e.g. The IUCr, Outreach, CIF and Associates) to make navigation easier within the huge content of the site.

With international travel severely restricted, the IUCr Finance Committee and Executive Committee (EC) had virtual meetings in March and August. Given the wide geographical distribution of EC members, meeting sessions were short and focussed, but we were very grateful to EC members for accepting

meetings at unsociable hours and to Sven Lidin, IUCr President, for – as usual – keeping a fast pace through the agenda.

The IUCr made a modest profit last year. That makes three years in a row after a series of heavy losses. Our finances are still far from secure but are at least more robust than they were at the last Congress. I would like to thank everyone who sent me an estimate of the number of hours that they donated, without charge, to the Union in 2019. Those were of sufficient value to persuade the Swiss authorities not to require any tax to be paid for 2019. While our not-for-profit status is still recognised, Switzerland does require an annual declaration of donated hours before they will agree not to levy a tax. We are optimistic that another declaration will be necessary for 2020, but with global economies being ravaged by the pandemic, it is difficult to look any further with any confidence at this stage.

With most crystallographic meetings being postponed or cancelled this year, the Calendar Committee is busy revising its rules to allow virtual and hybrid meetings to be supported in future. A packed meeting calendar in 2021 will present challenges of its own, so the Committee aims to be as flexible and adaptable as budgets will allow.

The pandemic forced the Prague organisers to postpone the [Congress](#) until August 2021, but we hope that life will have returned to normal by then and that we can all get together to celebrate being able to get together (as well as the excellent science that you all do). The postponement of the Congress provides an opportunity for National Committees to modify or add to their nominations for IUCr Commissions and for the EC. It also gives more time for countries that are considering applying to join the IUCr, and the Executive Outreach Officer is already working closely (*via Zoom*) with at least one potential applicant. We would also like to thank the officials and members of the EC and the IUCr Commissions who agreed to add an extra year to their planned terms of office to take us through to the end of what will now be a quadrennium.

One of my bosses in my previous job earned a (literal) slap in the face by telling his boss that there was no such thing as a problem as they are all opportunities. Nobody wanted this opportunity, but the pandemic has demonstrated to anyone who cares to pay attention just how important science in general and crystallography in particular are to our society. We have been trying to keep track of the [contributions of crystallographers](#) to characterise and understand the functionality of SARS-CoV-2 and related viruses. IUCr Journals are offering [fast publication of relevant articles](#), which we expect to be published open access. Click [here](#) for free access to a special virtual issue presenting articles and abstracts on coronaviruses that have been published in IUCr journals, including Ted Baker's acclaimed Editorial. The [International Science Council](#) has provided links from their website to our *Newsletter* articles and website for the benefit of the members of other international unions and associations. When a vaccine is finally available, the contributions of crystallographers and other structural scientists around the world will have been a critical part of humanity's response to this terrible virus.

Finally, our thoughts turn to the crystallographers we have lost and to those of you who have lost loved ones during this dreadful year. Stay safe and keep well.

ASSOCIATES NEWS

IUCr Associates Programme renewals due

Alex Ashcroft



The provision of bursaries for young scientists to attend meetings is just one of the IUCr's good works made possible by IUCr Associates and other donors. The photo shows the presentation of the IUCr Travel Awards at [ECM32](#) in Vienna, Austria, in 2019. The ECM32 organisers had the novel idea to use children of attendees to present the awards at the closing ceremony. This young lady also did the honours with the IUCr Poster Prizes (see below).

The IUCr Associates Programme was launched at the IUCr Congress in Hyderabad in 2017. It was hoped that the Programme would both raise some money for the IUCr's good works and also provide more of a sense of community for those who chose to join. It cost USD 200 for three years, with a reduced rate of USD 60 being available for retired crystallographers, students and crystallographers in developing countries. We would like to express our thanks to those who have joined the Programme. For those who joined in 2017, renewal notices will be sent out shortly. Prices are unchanged for the next triennium. We have been surprised by how few Associates have used their membership benefits, so here is a reminder of some of the best ones:

1. A 50% discount off the purchase price of printed volumes of *International Tables* for personal use – do you have space on your shelf for the new [Volume H: Powder diffraction](#)? Or perhaps you never got around to getting the new edition of [Volume A: Space-group symmetry](#). [Volume I: X-ray absorption spectroscopy and related techniques](#) is due out next year and you can use the discount as many times as you like. Discounts are also available on other IUCr books and books from some other academic publishers.
2. Vouchers for six free downloads of articles from [IUCr Journals](#).

3. A 20% discount on the fee when publishing an article in an open-access IUCr Journal (**IUCrJ**, *Acta E* and *IUCrData*). Associates also currently pay a lower fee for publishing open access in the IUCr's hybrid journals.

Between 2017 and 2019, we estimate that the IUCr spent almost USD 1 million on outreach and education. This includes providing bursaries for young scientists to attend meetings, paying for Visiting Professors to attend schools and workshops, and President's Fund grants to allow financially disadvantaged crystallographers to attend the Hyderabad Congress. This figure does not include fee waivers that subsidise open-access publications from scientists in low-income countries or the cost of books and open-access vouchers provided as prizes at meetings. Those were worth more than USD 100,000 in the same period. Some of these good works are funded by the generosity of the Editors of IUCr Journals, some of whom donate a proportion of their honoraria to the [IUCr Outreach and Education Fund](#) or the [Crystallography in Africa](#) initiative, but the income from the Associates Programme has also been used to fund this.



Left: IUCr Travel Award recipients at ECM32, and right: IUCr Executive Committee member Wulf Depmeier and guest present the IUCr Journals Poster Prize (Applied Crystallography) to Raffael Rameshan (centre) (Technische Universität Wien, Austria).

I am proud of what the IUCr has achieved and very pleased with how my Associates Programme membership fee has been spent. I hope that those of you who have become Associates feel the same way.

If you would like to join the Associates Programme or to donate money to the IUCr, the links are here:

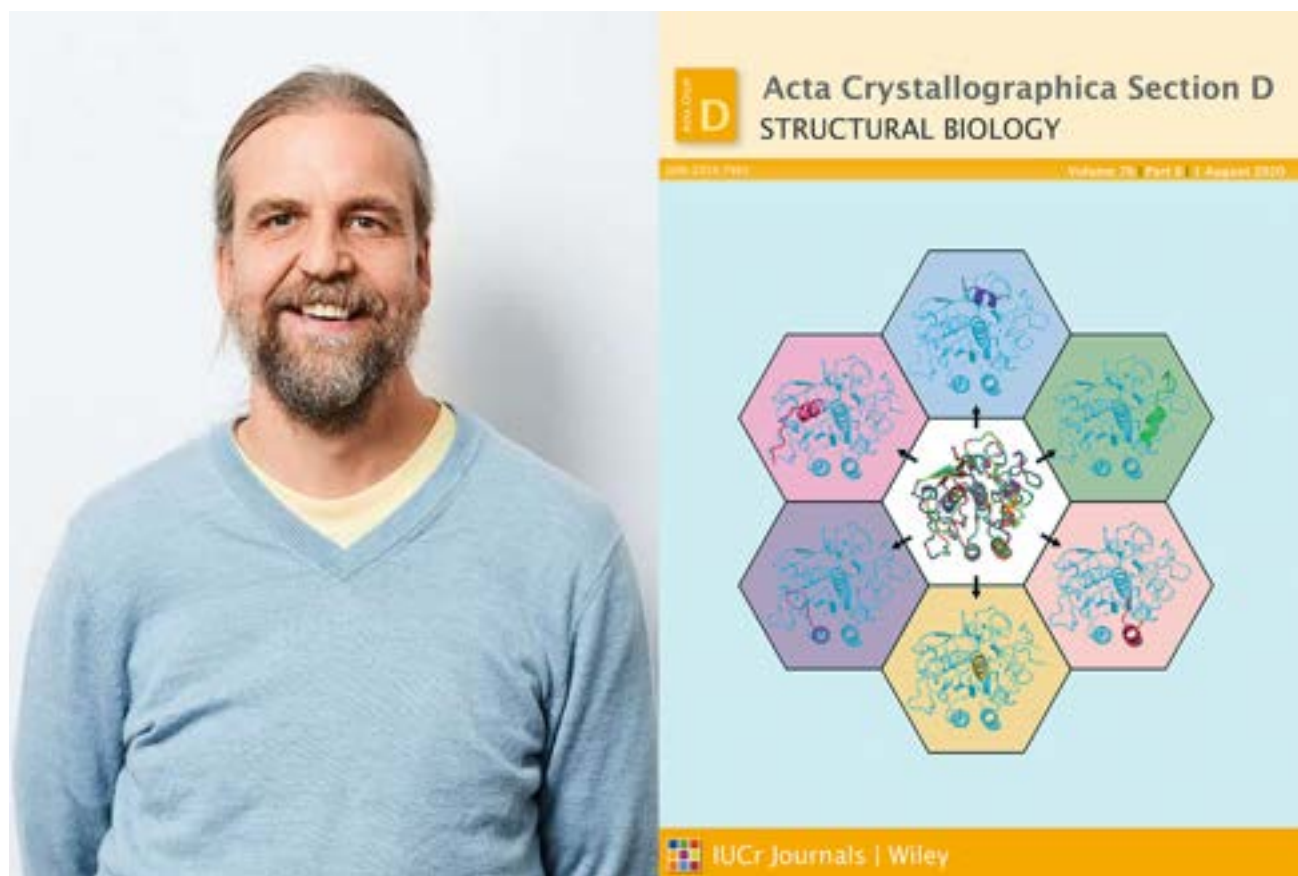
<https://www.iucr.org/people/associates/become>

<https://www.iucr.org/outreach>

IUCR JOURNALS NEWS

New Section Editor of Acta Cryst. D

Elspeth F. Garman Randy J. Read



Charlie Bond, the new Section Editor of *Acta Cryst. D*.

Professor Charlie Bond of the University of Western Australia has recently been appointed as a Section Editor of *Acta Cryst. D*.

Charlie started his academic career by studying Chemistry with Industrial Experience at the University of Manchester in the UK, staying there to complete a PhD in the group of Bill Hunter on the structure of the protein drug target, trypanothione reductase. After a postdoctoral fellowship at the University of Sydney with Mitchell Guss and Hans Freeman, he returned to the UK for several years as a BBSRC David Phillips Research Fellow and honorary lecturer at the University of Dundee. Since 2006 he has been a Professor at the University of Western Australia in Perth, where his group employs a broad range of techniques encompassing innovative research in biological chemistry, molecular biology and structural biology, relying on national facilities such as the Australian Synchrotron and the Opal Reactor.

His research particularly focuses on investigating biomolecular complexes and their interactions. To quote from his website: 'I want to understand how the spatial arrangement of biological molecules in complexes dictates their function. I am particularly interested in protein:nucleic acid interactions, and their functions in gene regulatory complexes in eukaryotes'.

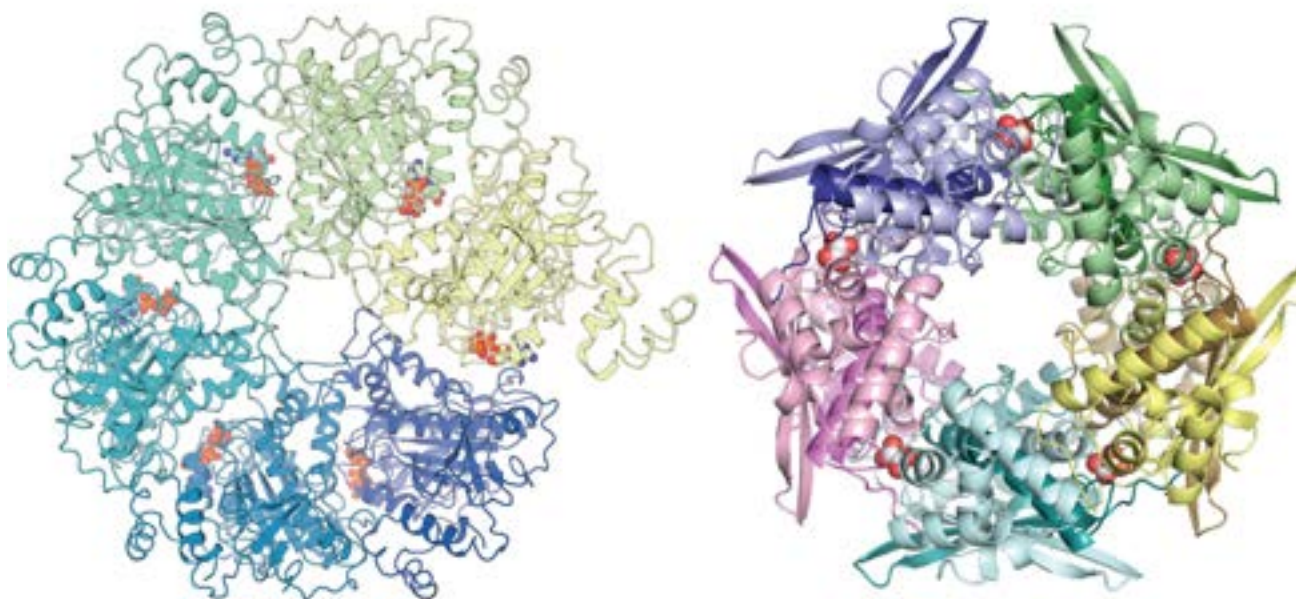
Charlie has been active as a Co-editor of *Acta Cryst. D* since 2011. The two existing Section Editors (Randy Read and Elspeth Garman) are delighted to welcome him to the team, and look forward to working with him to further development of the journal for the structural biology community.

This article was originally published in [Acta Cryst.](#) (2020). **D76**, 702.

EDITORIAL

Contamination or serendipity – doing the wrong thing by chance

Janet NewmanMark J. van Raaij



To contaminate – definition 2 in the Merriam-Webster (online) dictionary – is to ‘make unfit for use by the introduction of unwholesome or undesirable elements’, and a contaminant is then something that contaminates. As was pointed out in 2016 (Niedzialkowska *et al.*, 2016), the process of X-ray crystallography is rich with opportunities for contamination, and this can result in the production of an unexpected structure. A ‘contaminant’ in structural biology is generally ‘undesirable’ rather than ‘unwholesome’, as very careful and thorough analysis is required to deconvolute the unexpected results when a contaminant progresses through all the involved process of expression, purification, crystallization and structure determination. Two such examples are presented in this issue – a structure of the *E. coli* terminator protein Rho (Fan & Rees, 2020), and the structure of a cyanate hydratase from a *Serratia* strain of bacteria (Pederzoli *et al.*, 2020). In both papers, careful crystallography enabled the identification of the protein that resulted in crystals, in particular the use of rotation functions to identify unexpected non-crystallographic symmetry.

Given the development of tools to help identify contaminating proteins – *Contabase* and the associated *ContaMiner* (Hungler *et al.*, 2016), and the more recent *SIMBAD* tool (Simpkin *et al.*, 2018), why are contaminating proteins still an issue? One reason may be that the identity of purified proteins is not always checked by mass spectrometry or N-terminal sequencing and a band of the right size on a denaturing poly acrylamide gel is often taken to be sufficient evidence.

Another reason may be that novel contaminants are simply not presented as such; the authors embrace the serendipity and publish as if the structure was the intended goal – one of us has certainly been guilty of such an approach (Newman *et al.*, 2013). More interesting is the idea that every expression of a heterologous protein stresses the host in different ways, which can lead to the upregulation of different proteins, and thus a different protein background, even when using the same, well utilized expression system. So protein structures that are apparently unfortunate errors might provide insight into the mysteries of heterologous expression.

Finally, crystals forming from a mixture where the contaminant made up a tiny fraction of the protein present may be surprising to many, and is something to keep an eye out for (Fan & Rees, 2020). The possibility of *Serratia* contaminating an *E. coli* expression strain (Pederzoli *et al.*, 2020) was, for us at least, also an eye-opener – definitely something for all protein producers to be aware of and to try to prevent.

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This article was originally published in *Acta Cryst.* (2020). **F76**, 391.

Find a compilation of publications on contaminant protein structures and resources in IUCr journals [here](#).

EDITORIAL

Computational modelling as a tool in structural science

C. Richard A. Catlow

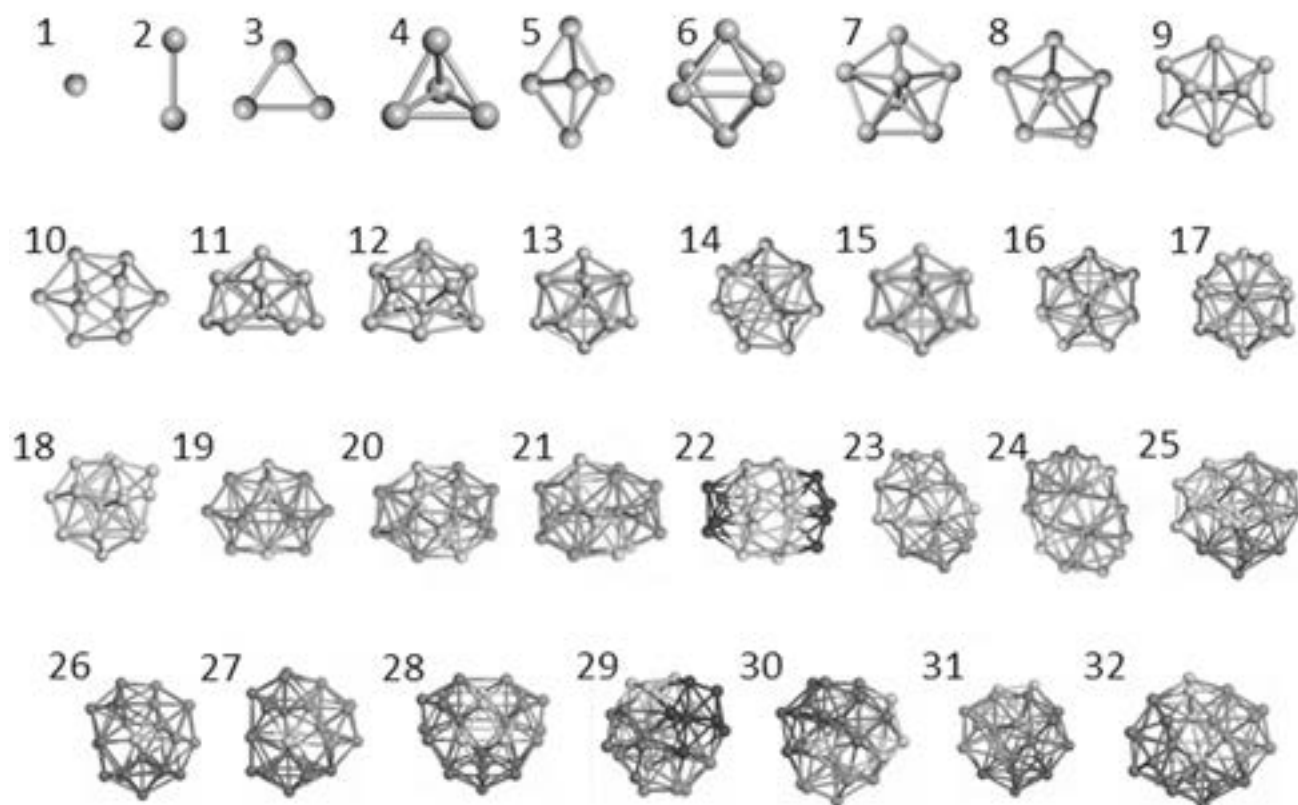


Figure 1. Predicted structures for titanium clusters with 2 to 32 atoms, after Lazauskas *et al.* (2018) (published by the PCCP Owner Societies).

Computational modelling is now integrated into almost all areas of science; and as well as being widely used for gaining insight and guidance in analysing and explaining experimental data, modelling has acquired an increasingly predictive capacity. This editorial will provide a brief review of its current status and role in structural science and will consider the likely future developments of the field. We focus first on our ability to model and predict crystal structures, after which we consider the challenges posed by disordered solids.

The use of computational methods in *modelling crystal structures* goes back many decades and in the 1970s and 1980s rapid progress was made with the use of methods based on interatomic potentials or force fields, coupled with energy minimization, to model accurately the crystal structures of a wide range of solids, both inorganic materials, including oxides, halides and silicates, and organic, molecular solids. These methods could be used to refine approximately known structures, as was also widely done in structural molecular biology. They could be enhanced by the use of molecular dynamical (MD) simulation methods and later by the use of density functional theory (DFT) based quantum mechanical methods, which as well as further refining crystallographic structures, generated models for the electronic structures of the materials. The article of Takada *et al.* (2018) provides an illustration of how MD methods

can be used to gain insight into complex structures, in this case, those associated with tridymite, while many examples of the applications of DFT techniques will be found in recent issues of **IUCrJ**.

Structure modelling, based on known structures, which may be approximate, remains a useful tool. Far more challenging, however, is *structure prediction* based simply on the composition of the solid. Indeed, a celebrated challenge was issued over thirty years ago in a 'News and Views' article in *Nature* by John Maddox, who provocatively wrote: '*One of the continuing scandals in the physical sciences is that it remains impossible to predict the structure of even the simplest crystalline solids from a knowledge of their composition.*' The field has responded well to the Maddox challenge over recent years and successful structure prediction has now been achieved for many classes of material, as discussed in the reviews of Woodley & Catlow (2008), Price (2018), Oganov (2018) and Woodley *et al.* (2020). The general approach is to navigate the configurational space defined by the structural parameters, using a rapidly computable 'cost function' which may be a simple energy evaluation; regions of low cost function are identified and the resulting structures may then be refined using energy minimization coupled with a more accurate energy evaluation employing a force field or quantum mechanical technique. The navigation of configurational space can use a variety of techniques and algorithms, including simulated annealing, genetic algorithms, and topological and molecular packing approaches.

An elegant recent example of the success of structure prediction in inorganic materials is provided by the work of Collins *et al.* (2017), who used a Monte-Carlo-based simulated annealing algorithm to predict a new structure in the complex phase field of an Y-Sr-Ca-Ga-oxide; the material was subsequently synthesized and the predicted structure confirmed experimentally. Prediction methods have also been successfully applied to organic materials, especially porous organic solids as illustrated by the recent work of Pulido *et al.* (2017).

Structure prediction is also extensively used in nano-science as reviewed by Catlow *et al.* (2010) for nano-clusters of inorganic systems. Recent work of Lazauskas *et al.* (2018) provides a good illustration of the application to metallic nano-clusters with the structures for titanium clusters with 2 to 32 atoms predicted by combining an MC search procedure using a force field with DFT refinement. The resulting structures are shown in Fig. 1.

An important recent development is the growing use of machine learning techniques, as discussed by Woodley *et al.* (2020). More generally, the field continues to take advantage of both developments in technique and algorithms and the continuing expansion of computer power. Crystal structure prediction is still far from routine, but it is an increasingly important tool in structural science. As structure prediction becomes more widespread, it will be essential that the metadata accompanying the structure make it clear whether the structure is experimentally determined, predicted or some combination of the two.

Turning now to *disordered* solids there are many challenges to both experiment and computation as shown by several articles in **IUCrJ** over recent years. The first concerns the structures and energies of defects in crystalline solids. Modelling of *point defects* in solids was indeed one of the earlier successes of computational condensed matter science, where work in the 1970s and 1980s using force-field-based methods was able to achieve good agreement between calculated and experimental defect properties, especially in inorganic materials. The field was extended to include more complex defect structures, including point defect clusters and line and planar defects, and it has continued to develop rapidly. Contemporary work still makes some use of forcefield methods, but is increasingly based on quantum mechanical methods using quantum mechanical/molecular mechanical (QM/MM) methods and periodic DFT techniques. Modelling is now an integral tool in the physics and chemistry of defective solids.

Heavily disordered solids including solid solutions and systems with high defect concentrations are attracting growing attention as again shown by articles over recent years in **IUCrJ**, and pose substantial challenges to theory and modelling. A common approach is to set up a supercell, aiming to model a disordered distribution within that cell. Realistic models may require very large cells and sampling of

large numbers of configurations, although these requirements can be reduced by the use of symmetry as in the widely applied site occupancy disorder (SOD) approach developed by Grau-Crespo *et al.* (2007). Monte-Carlo techniques including those available in the knowledge led master code (KLMC) approach developed by Woodley and co-workers (see e.g. Lazauskas *et al.*, 2017) also assist in modelling complex disordered solids, but the field is one of the most difficult and demanding in structural science.

Computational methods have for many years been used to construct models of amorphous solids. The general approach is to mimic the way by which glasses have traditionally been made, that is to quench from the liquid state. The process is simulated by a molecular dynamics ‘melt quench’ cycle in which MD is used to simulate the melting of the crystalline form of the material, followed by rapid cooling in which the system freezes into the amorphous state. Due to limitations in the time sampled by even the most ambitious MD simulations, the method has the problem that the timescale of the MD quench is far shorter than that of an experimental quench. A number of approaches have been developed to mitigate this problem and the MD modelling of disordered materials has enjoyed considerable success, although challenges remain. A detailed discussion of the field is given in the monograph of Massobrio *et al.* (2015); and there is no doubt that the structural science of amorphous solids will continue to gain valuable input and insight from modelling techniques.

The capabilities of modelling tools are advancing rapidly and the range and ambitions of applications will grow. **IUCrJ** will continue to welcome articles which develop and apply modelling techniques as a tool in structural science.

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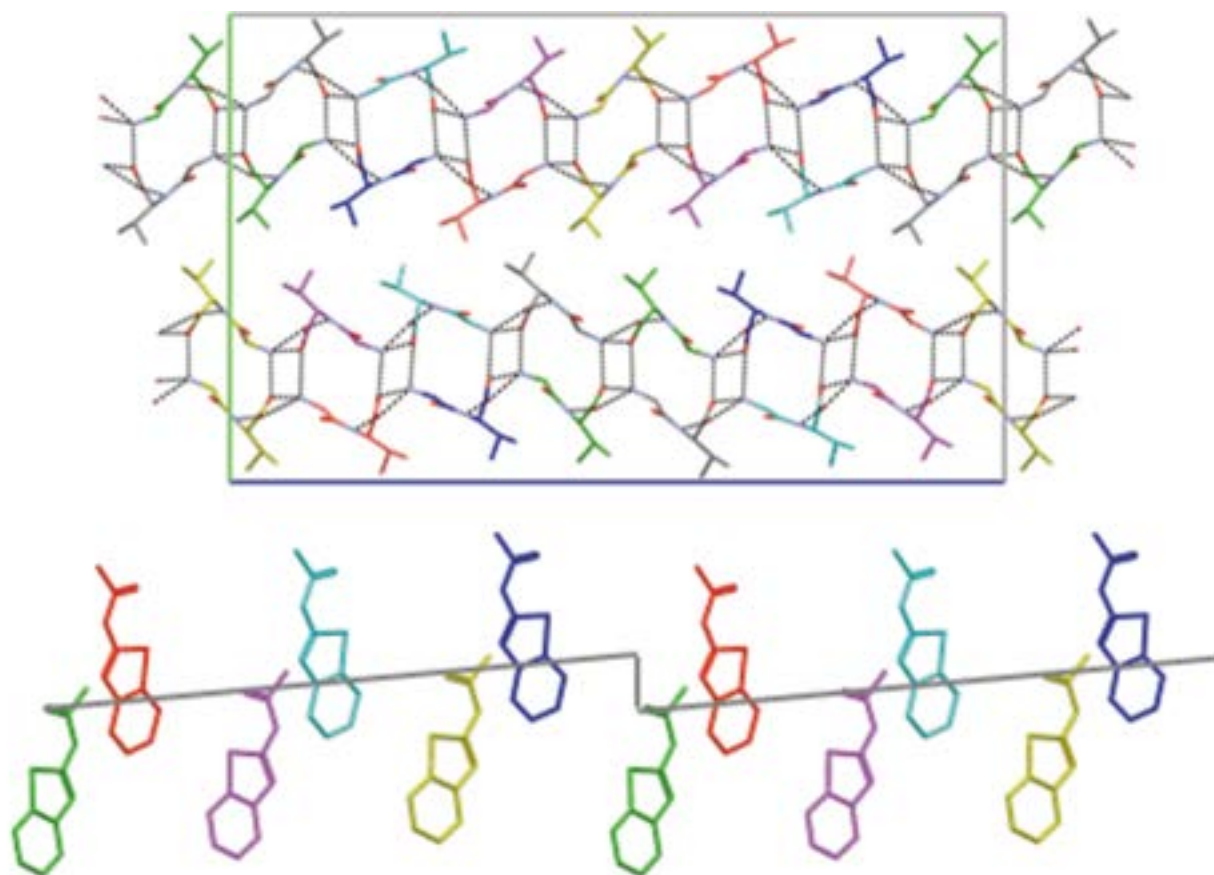
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COMMENTARY

Looking deeper into molecular structures with $Z' > 1$

Gervais Chapuis



In most crystal structure determinations with a given chemical composition, we expect that the number of formula units contained in the unit cell (Z) is at most equal to the multiplicity m of the general position, a fundamental characteristic of the corresponding space group. If this is the case, Z' which is equal to the quotient Z/m is one. Under such premises and if we are dealing with a molecular compound, finding the atomic structure and relative position of a single molecule is sufficient to characterize the entire crystal structure owing to the properties of the space group symmetry. However, cases may occur when Z' becomes an integer larger than one which often leads to interesting discoveries, for example, the existence of structural modulations.

The article by Brock & Taylor (2020) specifically deals with the identification of such cases by systematically scanning the organic structures stored in the Cambridge Structural Database. More specifically, the study focuses on translationally modulated molecular crystals which do occur, sometimes frequently, depending on the value of Z' . Each one of the Z' molecular structures presents numerous ways to deviate from an average form. Four types can be distinguished namely *conformational*, *orientational*, *longitudinal* and *transverse*.

In order to systematically scan the full set of molecular structures contained in the Cambridge Structural Database, the authors designed an algorithm to scan a large number of possible directions in the crystal structure in order to identify additional translational periodicities allowing the acceptance of minor

deviations to be specified. The method is not always successful, and, in some cases, it has to be completed by visual observation.

The method proposed by the authors is certainly well adapted for a systematic search in a database of molecular structures and I consider it as complementary to another method which is also frequently used and based on the Fourier transform of the crystal structure, *i.e.* on the diffraction pattern of the structure. The intensity distribution of diffraction patterns is well adapted to identify any translational characteristic including approximate translations. Such a method has been used successfully, for example, by considering a family of inorganic compounds, scheelites, with many different periodicities where each member can be related to a *single* model based on a commensurately modulated structure (Arakcheeva & Chapuis, 2008).

The main interest in the search of any type of translationally modulated structures is that it reveals very subtle interatomic interactions which might not be obvious to detect. What are the main factors of structural modifications causing Z' to increase? Can molecular dynamical simulations reproduce such interactions? It appears that this is possible as shown, for example, by Pan & Chapuis (2005) provided that an adapted force field is selected.

There is another very interesting issue concerning very large Z' numbers which are not directly related to molecular structures but rather to inorganic or metallic structures under specific temperature or pressure conditions. Cases of structure with Z' reaching up to nearly 100 have been studied. Knowing that for metallic structures it is not uncommon to observe values of $Z' =$ [Image unavailable], one may wonder why a structure requires such a large number of independent atoms? After deeper studies it appears that the publishing authors have missed identifying the appropriate symmetries of the particular compound [see examples given by Perez-Mato *et al.* (2006) or Arakcheeva *et al.* (2017)].

The study of molecular structures presented by Brock and Taylor with Z' larger than a specific limit reveals the complexities of intermolecular interactions in crystals. The analysis of the results indicates various possible mechanisms of molecular distortions which will be very helpful for a deeper analysis of the molecular dynamical mechanisms that come into play. The task is certainly not simple but a combination of various methods, *i.e.* crystallographic analysis both in direct and reciprocal space combined with molecular dynamical simulations, would probably be the best bet for a deeper understanding of the interactions.

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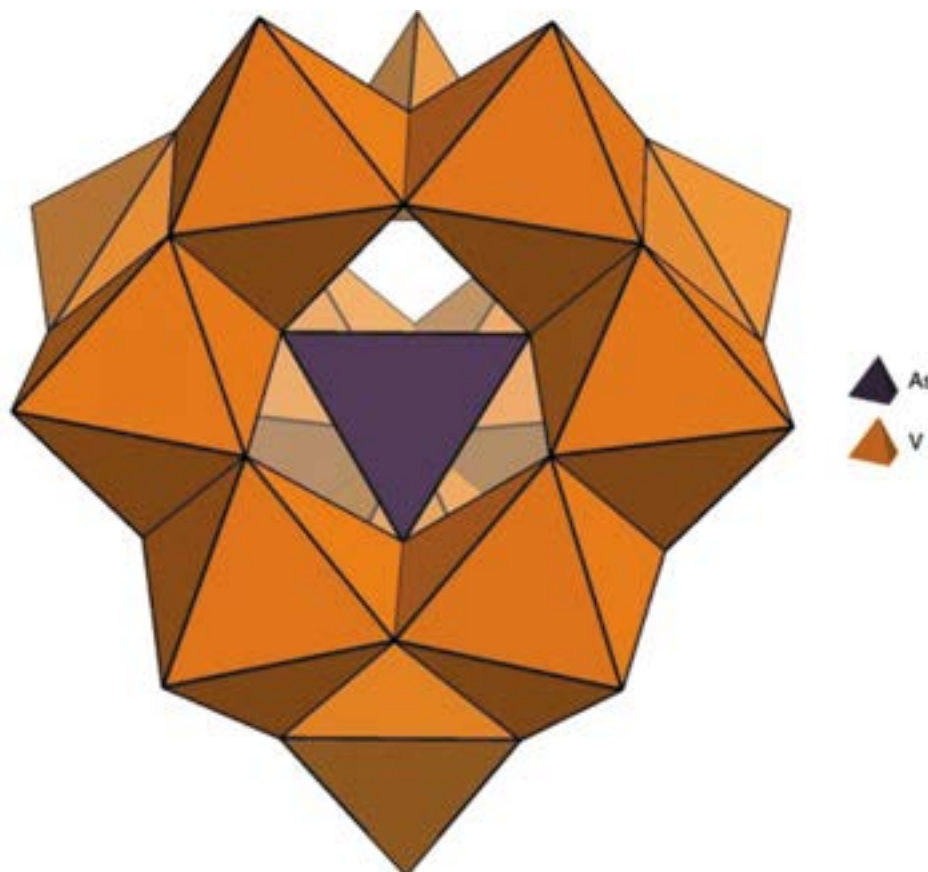
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COMMENTARY

Complex minerals preserve natural geochemically important nanoscale metal oxide clusters

Peter C. Burns



In his article, Krivovichev (2020) examines the emerging class of polyoxometalate-bearing minerals and the origins of their unusual complexity in terms of information content. The 42 minerals in this class constitute less than 1% of recognized mineral species, but their descriptions mostly require the current generation of X-ray diffractometers, and it is likely that many more will be discovered by new mineral hunters in the future. Indeed, this is a rapidly growing class with 34 (81%) of its species described within the past two decades.

The average complexity of mineral crystal structures is about 220 bits per unit cell, and all 42 polyoxometalate-bearing minerals exhibit much higher than average complexity owing to the presence of nanoscale metal oxide clusters in their structures. The information content of the most complex of these, the uranyl carbonate ewingite, is more than 100 times higher than average. The structure of ewingite is also the most complex known mineral structure.

In 1783, Carl Wilhelm Scheele provided the first surviving written report of blue waters in the Idaho Springs (USA) region, but undoubtedly these had been observed previously. The blue waters are thought to be colored by soluble molybdenum oxide clusters ($\text{Mo}_3\text{O}_8 \cdot n\text{H}_2\text{O}$) that crystallize as ilsemannite (and related species), which was first described in 1871. The mineral is inadequately characterized even

today, in part because of its poor crystallinity and likely corresponds to several different species containing a variety of molybdenum oxide clusters that are examples of natural polyoxometalates. Dissolution of so-called ilsemanite in water produces a greenish-blue solution that later deepens to a typical molybdenum blue.

Under the right conditions, metal oxide clusters spontaneously self-assemble in aqueous solution. These anionic clusters can contain several hundred atoms and have dimensions ranging up to several nanometres. These have been extensively studied by inorganic chemists, who have revealed the impressive range in cluster structures and compositions. Owing to their lower charge densities and well defined structures, metal oxide clusters behave very differently in solution than simpler metal-bearing species, and high solubility is a hallmark of such clusters. There are many potential and realized applications of metal oxide clusters, and they are excellent model systems for studying structure–composition–size–property relations.

Differences in chemical bonding distinguish self-assembling metal oxide clusters in aqueous solutions that persist at the nanoscale, as compared to nucleation of nanoscale clusters that continue to grow and become crystals. Polyoxometalates are generally defined as the class of metal oxide clusters that contain multiple bonds between metal cations and oxygen. Such bonds are common in the case of d^0 transition metals of groups V (V^{5+} , Nb^{5+} , Ta^{5+}) and VI (Mo^{6+} , W^{6+}), as well as the actinides U, Np and Pu in their pentavalent and hexavalent oxidation states. The doubly or triply bonded oxygen atoms tend not to bridge to other metal centers and instead serve to stabilize the surface of the polyoxometalate. As such, polyoxometalates are inherently nanoscale materials and they have no macroscale analogs. Other types of nanoscale metal oxide clusters have surfaces that are stabilized by different chemical features, including protonation of oxygen atoms and capping by organic ligands.

Synthetic transition metal and actinide-based polyoxometalates have been extensively studied both in solution and the solid state. These clusters have been definitively demonstrated to self-assemble in solution, where they can persist indefinitely, or crystallization can be induced by evaporation from solution or various other methods. It is particularly important to recognize that such clusters can form and persist in natural aqueous solutions, where they can be highly soluble and mobile in geochemical systems. Minerals sometimes form that reveal and record their presence, but it is probably much more common for such clusters to enhance metal transport in a geochemical environmental system and then vanish without a trace. Indeed, the occurrence of polyoxometalates in natural systems presents a substantial challenge for geochemical models that traditionally do not account for nanoscale metal oxide clusters in aqueous systems, especially as it pertains to the mobility of these metals. Their solubilities are often much higher than those of simpler metal oxide complexes owing to their lower charge densities.

Crystallization of polyoxometalates and other types of metal oxide clusters in nature produces minerals with higher than normal complexities (information content). These minerals also are dominantly of lower-temperature origin, which in general tends to result in more complex structures. All but two of the polyoxometalate-bearing minerals form in aqueous systems, with notable exceptions that crystallize directly from volcanic gas.

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COMMENTARY

Towards the automation of in situ experimental phasing

Dorothee Liebschner

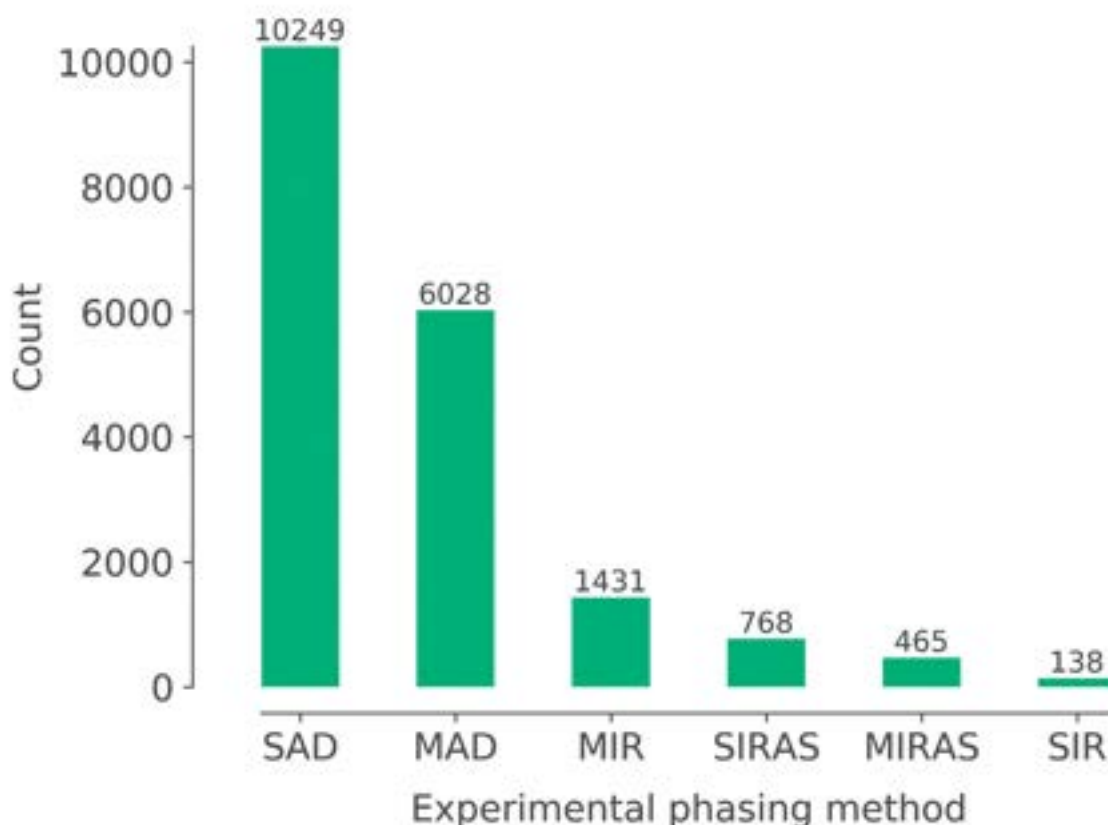


Figure 1. Count of experimental phasing methods for X-ray models deposited in the PDB, in descending order. The counts are obtained from the RCSB advanced search, so they depend on correct annotations in the metadata. Not shown: RIP phasing, 7 entries. Other phasing methods: MR, 104,673 entries; direct methods, 166 entries (search for keyword and resolution better than 1.4 Å).

The predicament of a diffraction experiment lies in the loss of phase information. Fortunately, it is possible to recover phases, either experimentally or through computations, by assuming some prior knowledge about the molecular structure (*i.e.* the electron density). Three methods exist to recover phases from a diffraction experiment: (1) direct methods (Karle & Hauptman, 1956), which rely on phase relationships that can be formulated by assuming the positivity and atomicity of the electron density. (2) Molecular replacement (MR) (Rossmann, 1972), which is based on the observation that a previously known structure can provide initial phase estimates for the new structure. (3) Experimental phasing (Fig. 1), which exploits the properties of a few special atoms in the macromolecule, such as anomalous scattering, a large number of electrons, or a combination of both (reviewed by Dauter & Dauter, 2017). Direct methods can be only applied if the resolution of the diffraction data is very high (better than ~1.2 Å), which only occurs in exceptional cases for macromolecular crystals. MR is widely applied, thanks to well established algorithms and protocols, and the availability of a trove of models in the Protein Data Bank (Berman *et al.*, 2000). However, it may happen that no known structures can be found that provide

good enough phase estimates for the new structure. In this case, the only possibility is to resort to experimental phasing.

The basic idea of experimental phasing is to locate the position of a subset of atoms ('marker atoms') that have particular properties. The marker atoms can be purposely incorporated or natively present in the sample. If the marker atoms have many electrons, such as heavy-metal salts or metal clusters, isomorphous replacement tries to detect the difference in amplitudes for the native and the derivative crystal. The approach can be done with one (SIR) or several derivatives (MIR). The intensity differences can reach as much as 15–25% (Crick & Magdoff, 1956), but incorporating the marker atoms may also cause non-isomorphism. This can result in similar changes of intensity, therefore complicating the phasing process. Other challenges of SIR/MIR are the toxicity of some heavy atoms, finding the appropriate marker atom type, and the deterioration of the crystalline order when the heavy atoms bind to the macromolecule.

Another experimental phasing approach exploits the difference in intensities between reflections related by Friedel's law for anomalous scatterers, such as selenomethionine. The approach can be done at one (SAD) or several (MAD) energies near the absorption edge of the marker atom. As a complete SAD/MAD dataset can be collected from a single crystal, isomorphism is less of a problem than for SIR/MIR. However, the anomalous differences in intensity are much smaller, so the experimental data have to be measured very accurately.

The single and multiple isomorphous replacement with anomalous scattering methods (SIRAS and MIRAS) combine the heavy-atom and anomalous scatterer approaches by also using the dispersive signal of the heavy atom.

While the above-described methods are well established, they still face technical and computational challenges. Therefore, a significant amount of effort is being directed to achieve advances in experimental phasing. For example, SAD phasing is now increasingly used with sulfur and ions that can exist natively in macromolecules (Rose *et al.*, 2015). Furthermore, it was shown that combining data sets from multiple crystals can improve the chances of determining the substructure (Liu *et al.*, 2011). Some synchrotron beamlines are specifically designed to collect data near the absorption edge of sulfur (Wagner *et al.*, 2016), or to collect accurate and high-multiplicity data (Olieric *et al.*, 2016). A new metric assesses the potential of SAD data to successfully solve the structure (Terwilliger *et al.*, 2016a,b). Recently, a new approach to experimental phasing was suggested by Lawrence and colleagues in an *Acta Cryst. D* article (Lawrence *et al.*, 2020). The procedure makes use of robotics to automatically soak hundreds of samples in heavy-atom solutions, producing isomorphous derivative crystals. Partial diffraction data are collected *in situ* at room temperature (RT) and combined to maximize the anomalous signal.

Lawrence *et al.* proceeded as follows to demonstrate their approach. Crystals of tetragonal lysozyme and proteinase K were prepared in 96-well sitting-drop plates with a crystallization robot. Some wells containing crystals were automatically soaked with halide (NaBr, KBr, NaI, KI) and heavy-metal solutions [$\text{K}_2\text{Pt}(\text{NO}_2)_4$, $\text{KAuCl}_4 \cdot \text{H}_2\text{O}$, K_2IrCl_6 , $\text{SmCl}_3 \cdot 6\text{H}_2\text{O}$] by using a liquid handler. A subset of native and derivative crystals was manually cryo-cooled for control measurements at 100 K. To perform *in situ* data collection at RT, the crystallization plates were directly mounted on a goniometer and 21–116 partial data sets were collected on different crystals. Native data sets were collected around 12 keV incident X-ray energy while the energies for the derivative crystals were adapted to the type of heavy atom. Phasing was attempted with the SAD and SIRAS methods. Phasing was considered a success if three indicators were successful: anomalous signal strength (as expressed by d''), substructure solution and the fraction of residues that could be built automatically.

For the 100 K control measurements, phasing of lysozyme works in all cases for both SAD and SIRAS. Proteinase K was successful in four cases for SAD and in four cases for SIRAS. At RT, lysozyme phasing is successful in half of SAD and SIRAS cases. Proteinase K only works for the gold derivative. Generally,

SIRAS, which can solve the phase ambiguity for the substructure, results in a larger fraction of residues built.

Several observations can be made from the results. Isomorphism, as measured by the associated unit-cell variability, is markedly better at RT than at 100 K. As this new phasing approach relies on isomorphism, it corroborates the choice of performing the experiments at RT. Anomalous difference maps show clear peaks for at least a fraction of marker atoms. This means that the soaking protocol resulted in binding, which is a critical prerequisite for the method. Crystal size influences the phasing success, as showed by the results for the small proteinase K crystals ($10 \times 10 \times 10 \mu\text{m}$). Combining a large number of data sets may improve phasing outcome. The heavy-atom substrates have different propensities to bind to the macromolecule. Therefore, using a combination of substrates provides the largest chances of success that one may bind to the sample.

The high-throughput phasing method devised by Lawrence *et al.* will certainly be helpful for the macromolecular crystallography community as it reduces human intervention in the sample preparation process to a minimum, therefore increasing the chances of producing isomorphous crystals in reproducible conditions. This is advantageous for both SIRAS, which relies on isomorphism, and SAD, which benefits from it when data sets are combined from different crystals. Using two phasing methods, including one that breaks the phase ambiguity, increases the chance of phasing success. The high-throughput approach may either provide a phasing dataset or, if phasing was not achieved, it may help reveal promising conditions that can be further optimized. The authors suggest that the method may be also extended to serial crystallography. While some limitations exist, for example the *in situ* data-collection method will be challenging for low-symmetry space groups and suffers from higher background noise from the crystallization plate (thus reducing the achievable anomalous signal), the high-throughput phasing method has the potential to greatly facilitate heavy-atom phasing experiments.

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COMMENTARY

Electrons receive individual treatment with electron-event representation

Radostin Danev

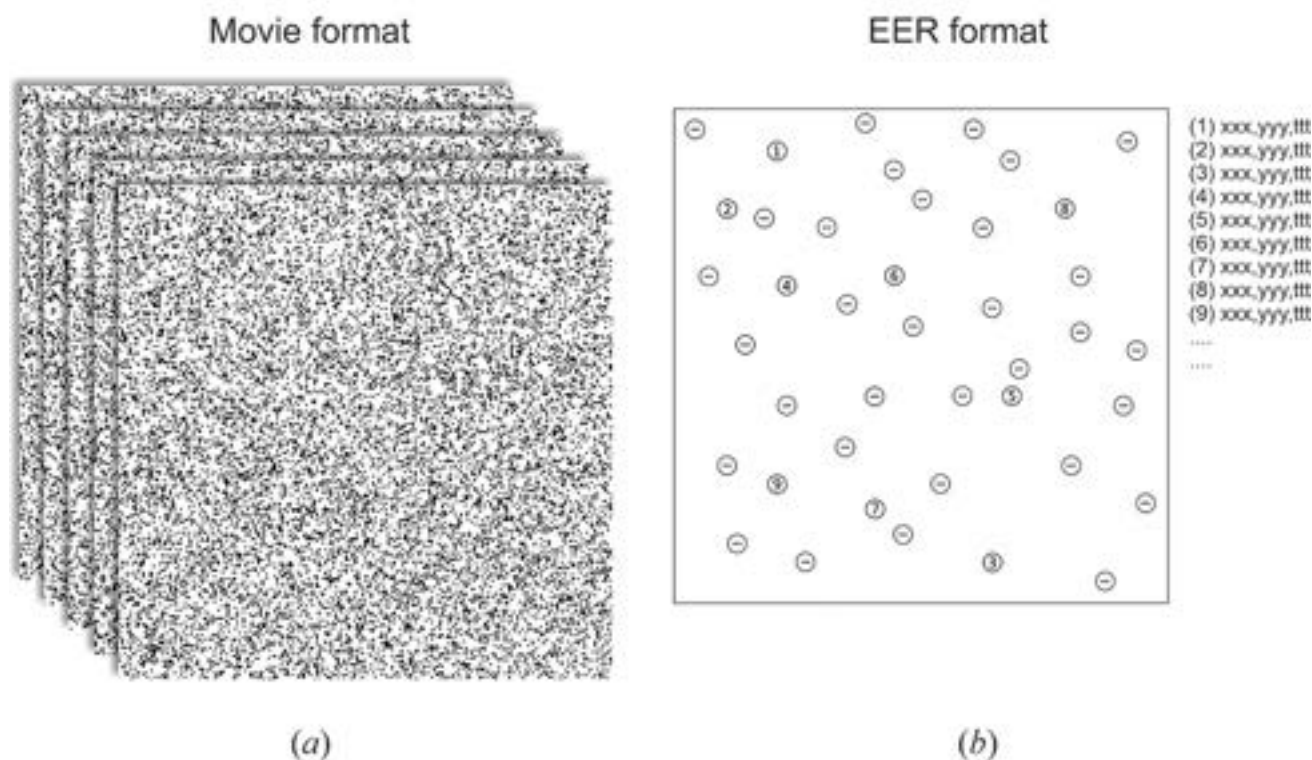


Figure 1. Illustrative comparison of (a) the current movie recording format and (b) the newly developed electron-event representation (EER) format. In the movie format, electron counts are accumulated in fractions of predefined time length that are stored as an image stack. The fraction length must be decided before the experiment and determines the shortest time interval at which beam-induced motion correction can be performed during data processing. Shorter fractions allow finer sampling but also increase the movie file size, necessitating a practical compromise with the fraction length. In the EER format, each electron is recorded with its spatial coordinates and the time of detection. The spatial coordinates have subpixel accuracy with fourfold super-sampling, which allows recovery of information beyond the physical Nyquist periodicity of the detector. During processing, the time interval for beam-induced motion calculations can be selected arbitrarily and optimized for best performance.

Up until a decade ago, photographic film provided the best performance for the recording of cryo-electron microscopy (cryo-EM) images. Digital cameras using a phosphor scintillator have also been available since the late 1990s, but despite being more convenient to use their signal-to-noise characteristics were significantly inferior to those of film. Irrespective of their differences, both recording methods were far from the theoretically achievable performance and limited the typical resolution of cryo-EM reconstructions to a ‘blobology’ (~ 10 Å) level. The inadequacy of these legacy image capture methods was resolved around 2012 with the first commercial introduction of direct electron detectors

(DEDs). Together with substantial advances in image processing algorithms, these new cameras played a fundamental role in the great leap in cryoEM performance.

As the name suggests, DEDs detect electrons through their direct interaction with the active silicon layer of the camera chip (McMullan *et al.*, 2016). They are based on CMOS technology that gives them radiation resistance and fast readout speeds. Unlike previous methods that recorded a single integrated image, DEDs are read out continuously during the exposure with a frame rate of a few hundred frames per second. Each frame contains a small number of incident electron events that are sufficiently dispersed to allow on-the-fly numerical identification and localization of individual electrons. The process is known as ‘electron counting’ and virtually eliminates detection noise, resulting in a superior signal-to-noise ratio. Furthermore, the localization of electron events can be performed with sub-pixel accuracy to extract information beyond the physical Nyquist frequency of the detector. The current approach for recording of the counted electron data is to accumulate the counts from several frames on an image grid and store it as an ‘exposure fraction’ in a movie. The pixel dimensions of the fraction are either the same as the detector or two-times oversampled for the so-called ‘super-resolution’ mode. The number of detector frames that are accumulated into each fraction is a parameter that must be decided before the experiment and cannot be changed after the data have been collected. Smaller fractions and super-resolution sampling can produce higher quality results but also significantly increase the size of the recorded movies. Therefore, researchers must make a compromise by selecting recording parameters that will provide close to optimal results without requiring excessive data storage space. In some unfortunate cases, after processing the data the *a priori* parameter choice may turn out to have been suboptimal, but apart from performing another experiment there is no way to correct it.

In a recent **IUCr** paper, Guo and colleagues (Guo *et al.*, 2020) present a new data recording and storage format for direct electron detectors called ‘electron-event representation’ (EER). Instead of recording movies, it captures each individual electron event and saves its coordinates in (x, y, time) space (Fig. 1). Consequently, the EER method preserves the spatial and temporal information for every electron and resolves completely the compromise between information retention and data size that is currently imposed by the movie recording format. Furthermore, EER uses fourfold spatial supersampling which allows it to capture high-resolution image components beyond the physical Nyquist periodicity of the detector, with sufficient signal-to-noise ratio to be usable in cryo-EM reconstructions. The authors provide an experimental demonstration with an apoferritin test sample that has reached a resolution 1.2 times the Nyquist frequency. Having good information preservation up to and even beyond Nyquist will allow researchers to comfortably collect data at lower microscope magnifications that give a larger sample area field of view, without high-resolution signal loss. This will increase the number of particles per image or the captured cellular area in cryo-tomography and boost the experimental throughput. The complete preservation of temporal information will also improve the performance by allowing finer sampling and interpolation on the single frame level during the beam-induced motion correction step of data processing. This will provide means for recovering a much larger portion of the high-resolution information that is present only in the very beginning of the exposure, before radiation damage of the sample has progressed, but also when the majority of beam-induced motion of the specimen is taking place. Because the EER format contains a complete representation of the electron events, experimentation and optimization of the motion correction fractionation parameters can be performed freely during data processing.

EER is another significant step in the development of cryoEM detector technology. It removes experimental restrictions and improves detector performance while also freeing researchers from mandatory data reduction decisions that had to be made with previous recording methods.

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COMMENTARY

The crystallography of Pluto

Christoph G. Salzmann Alexander Rosu-Finsen



Far beyond the realm of the mighty gas giant Neptune lies the icy world of Pluto. Originally believed to be an inactive and desolate dwarf planet at the outer rim of our Solar system, the New Horizons spacecraft recently revealed Pluto to be a 'scientific wonderland' with complex surface geology (Moore *et al.*, 2016; Hall, 2020) and atmospheric chemistry (Wong *et al.*, 2017). Writing in **IUCrJ**, Maynard-Casely and co-workers have now investigated two of the most abundant Plutonian minerals, solid nitrogen and methane, with powder neutron diffraction (Maynard-Casely *et al.*, 2020). The new results on the thermal-expansion properties, phase-transition behaviours and crystal structures of these materials will be key to understanding the active geology of our distant neighbour. This work also represents an important contribution towards advancing the emerging field of 'small-molecule geology' which is concerned with materials that are gases or liquids under Earth conditions but rock-forming minerals at greater distances from the Sun.

The surface of Pluto is a sight to behold. Rugged mountain ranges taller than Mount Everest give way to cracks deeper than the Grand Canyon and flat plains such as Sputnik Planitia which is part of Pluto's famous 'heart' region shown in Fig. 1(a) (Moore *et al.*, 2016). Solid nitrogen has been suggested to be the dominating mineral of this plain and fascinating polygonal surface patterns indicate active convection processes (Grundy *et al.*, 2016). The crystal structure of β -nitrogen displays orientational disorder of the N_2 molecules which are arranged in a hexagonal close-packed fashion [see Fig. 1(b)] (Streib *et al.*, 1962; Press *et al.*, 1982). This makes β -nitrogen a so-called 'plastic' phase which is a class of mechanically soft materials and therefore consistent with the convection processes of Pluto's plains. Maynard-Casely and co-workers present accurate density data of β -nitrogen and follow the phase

transition to α -nitrogen which is the stable phase below 38 K (Maynard-Casely *et al.*, 2020). In α -nitrogen, the nitrogen molecules display defined orientations and the authors now show that its crystal structure is best described by the $Pa\bar{3}$ space group thereby resolving a long-standing debate. The phase transition from β - to α -nitrogen takes place in a temperature range relevant for Pluto, and it can be speculated that the associated density change and most likely hardening of the material are important factors for Pluto's glaciology.

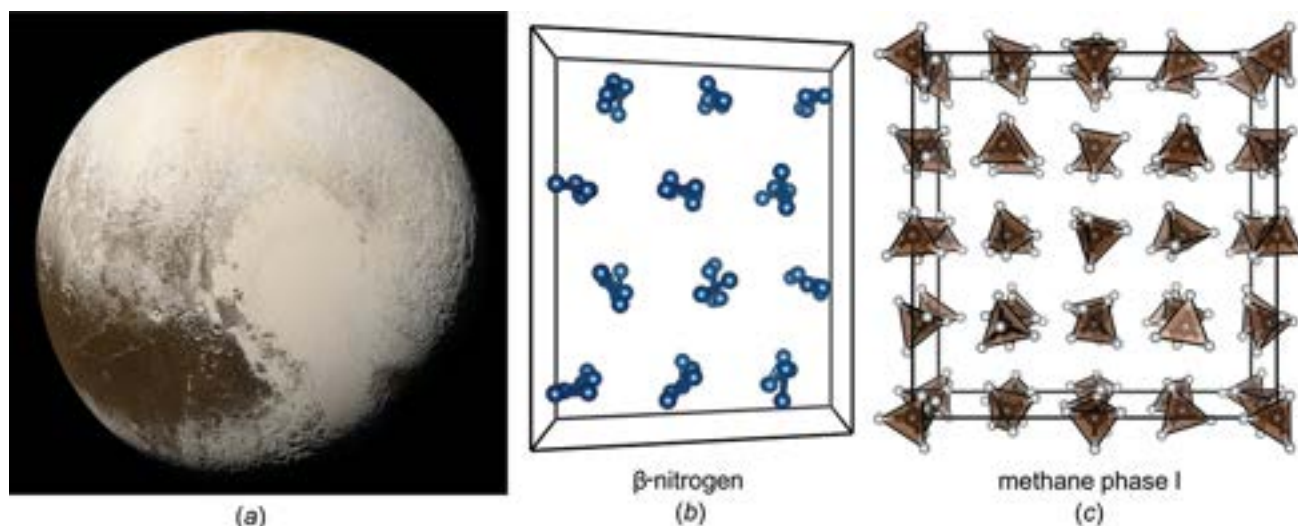


Figure 1. Pluto and the crystal structures of two of its most important minerals. (a) Photographic image of Pluto taken by the New Horizons spacecraft (Source: NASA/Johns Hopkins University Applied Physics Laboratory/Southwest Research Institute/Alex Parker. Published: July 23, 2018). (b, c) Crystal structures of β -nitrogen (Streib *et al.*, 1962, Press *et al.*, 1982) and methane I (Press, 1972) shown with random orientations of the N₂ and CH₄ molecules, and using 3x3x2 and 2x2x2 supercells, respectively.

Solid methane is expected to exist as phase I on Pluto which is, just like β -nitrogen, a plastic phase with orientational disorder of the CH₄ molecules that are packed in a face-centred cubic structure [see Fig. 1(c)] (Press, 1972). Again, Maynard-Casely and coworkers determined accurate density values for methane I which is, due to its high hydrogen content, a significantly lighter material than solid nitrogen. To their credit, the work was carried out with protiated methane, the form of methane expected to exist on Pluto, and not the deuterated analogue (CD₄) which would have offered tremendous advantages from the neutron diffraction point of view. Although not relevant for Pluto, they also followed the phase transition to methane II at low temperatures and observed hints of the intriguing phenomenon of negative thermal expansion. Above 65 K, they found that methane I transforms from a fine powder to large crystalline grains. Skyscraper-sized shards on Pluto are thought to consist of solid methane (Hall, 2020) and the observed changes in crystal size upon heating may provide an explanation for their formation.

Water ice is another important mineral on Pluto. Unlike solid nitrogen and methane, its density changes very little in the temperature range relevant for Pluto (Fortes, 2018) and it is a much harder material due to hydrogen bonding between the H₂O molecules (Salzmann, 2019). Hence, water ice is Pluto's 'bedrock' material and the major constituent of its tall mountain ranges (Grundy *et al.*, 2016). The likely form of water ice to exist on Pluto is the familiar hexagonal ice Ih. However, it has also been speculated that the ferroelectric low-temperature phase ice XI may exist (Fukazawa *et al.*, 2006).

Future work will focus on accurately measuring the mechanical properties of Pluto's minerals. Moving beyond the traditional fitting of Bragg diffraction data, total scattering studies and the analysis of pair-distribution functions can be expected to provide detailed insights into the local structures of the orientationally disordered nitrogen and methane phases. The interplay and mixing of the various minerals will need to be investigated in more detail as well. This will include the formation of solid solutions and the formation of clathrate hydrates in which cages of water molecules trap guest species

such as nitrogen or methane molecules. Most recently, it has been suggested that a layer of clathrate hydrates may provide the thermal insulation required to stabilize a subsurface ocean on Pluto (Kamata *et al.*, 2019). Pluto clearly still harbours many secrets and following the work of Maynard-Casely and co-workers, crystallography will certainly continue to be a major tool for understanding its geology. But also, considering how long it takes to reach Pluto, we should really send another spacecraft very soon to further explore this fascinating world.

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OUTREACH

A crystal growing competition at home - outreach activities during lockdown

Ivana Aguiar, Natalia Alvarez, Isabel Galain, Romina Keuchkerian, Maia Mombru, Ivana Nunez, Mauricio Rodriguez, Leopoldo Suescun



Martina González (left), one of the first-place winners of the Desafío de los Cristales with her well-deserved mug and certificate, and some members of the organizing group in the closing Zoom meeting: Maia, Leopoldo, Isabel, Ivana A., Romina, Ivana N. and Natalia.

In February 2020, the group in charge of organizing the Crystal Growing Competition in Uruguay (Concurso Nacional de Crecimiento de Cristales, CNCC) was already preparing activities for the seventh edition [1]. As usual, planning started with brainstorming about how to obtain financial resources, depending on the budget as to what activities could be added or would be suspended, and which companies or organizations would be contacted for support. Activities were distributed among group members and letters of request for support from different organizations were written, as the school-year activities were starting in the first week of March [note that the school calendar runs from March to November in Uruguay (in the southern hemisphere)].

This planning, however, became redundant on 13 March when the government implemented a state of sanitary emergency [2] after the first four positive cases of COVID-19 were confirmed in subjects coming from abroad. This declaration included a voluntary lockdown and a cancellation of all public activities that would imply indoor gatherings. Among them, teaching activities at all levels were put on hold without a date for resumption.

After two weeks of general discomfort and some forceful adjustments to virtual teaching and *Zoom* meetings, the CNCC WhatsApp group became active again, with questions on what to do, if we should respond to the crisis in any form or if we should just shut down for the year. Luckily, by 28 March, brainstorming had produced some very feasible ideas, and the unbreakable spirit of the group prevailed over the difficulties brought about by the lockdown and the widespread uncertainty. Eventually, the idea to organize a fully home-based competition materialized.

The CNCC would become "CNCC - Desafío de los Cristales - desde Casa" (The CNCC Crystal's Challenge from Home) and would replace a month-long crystal growing activity mainly focused on the classroom with significant participation from teachers with a set of short activities that would only require home appliances and safe "chemicals" and that could be performed with the help of parents or older kids.



Electronic flyer for "CNCC - Desafío de los Cristales - desde casa".

From 28 March to 7 April all the organizers performed home experiments with sugar (sucrose) and table salt (sodium chloride) in order to define challenges that were to be performed by the general public in one week and which could be evaluated only on the basis of pictures. By 15 April, six challenges had been planned, including photography of crystals, salt and sugar crystal growing, identification of periodic patterns at home and a Q&A series, with the aim to cover at least 2 or 3 months of (at that time expected) school closure.

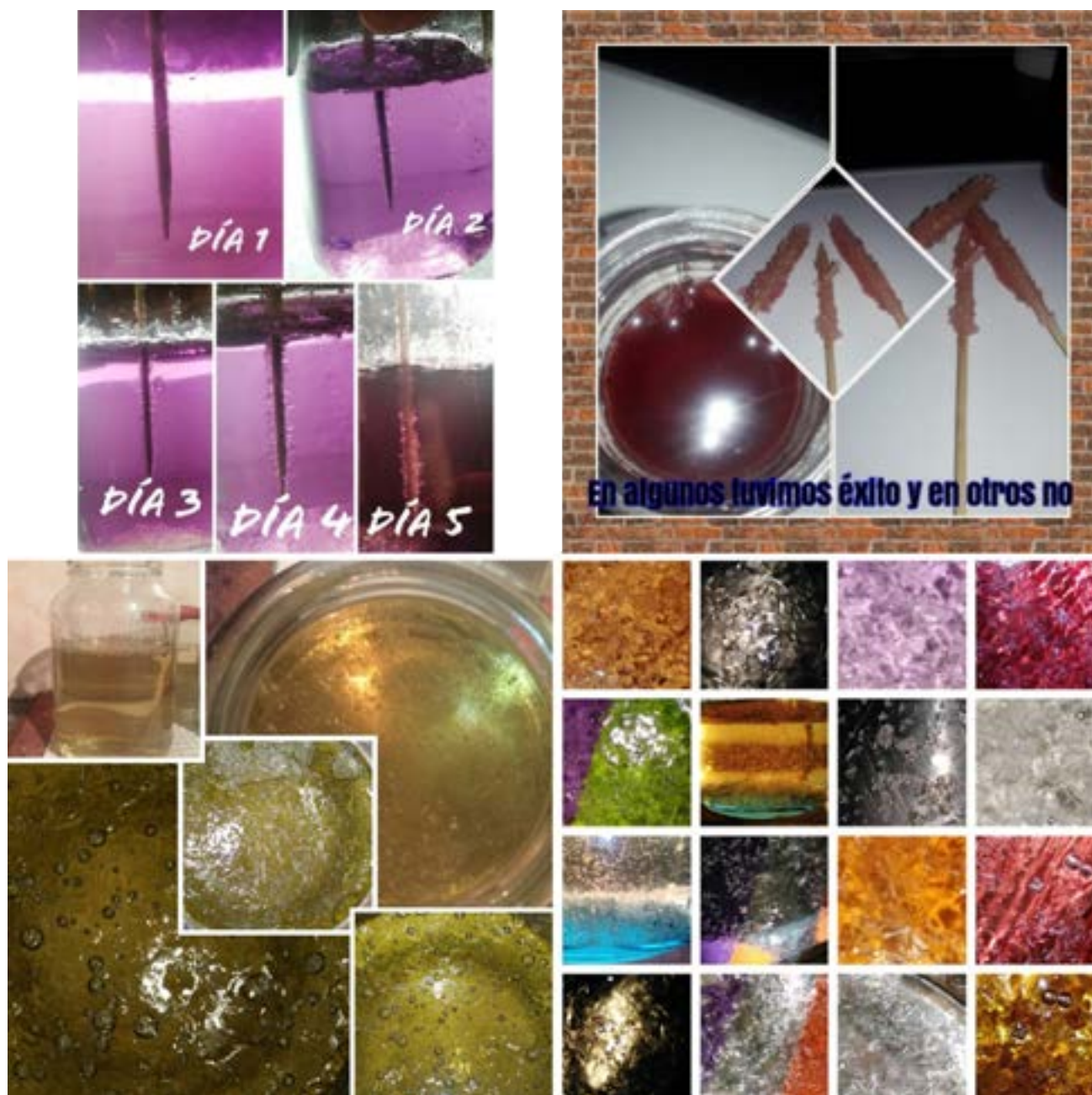
The new Desafío de los Cristales started on 20 April and consisted of two-week long activities that would be performed by participants at home, and their results would be submitted to the organizers in the form of pictures or through social media (Instagram @CNCCfquy), email (cnccfquy@gmail.com) or "plataforma CREA" [6], the platform for teaching resources of the Public Education Administration (ANEP) [7] of Uruguay to which all public and many private schoolchildren have access.

The organization counted on the widespread use of smartphones and laptops with a camera (distributed by the government to 100% of public school students aged 5–18 years old through an OLPC-like program called Plan Ceibal [3,4]) and a more than 90% smartphone/internet-access coverage of the country [5], which allowed every participating child/adult to interact through a web browser.

The challenges, available at [8], are listed below with some of the best pictures received from the participants:



#1 Taking pictures of crystals available at home and presenting them in a fancy way (where students learned that glass products do not qualify as crystals); photos/collages by Abigail Algibar (top left), Gabriel Musso (top right) and Samira Cabrera (bottom).



#2 Growth of colored sugar crystals by seeding, where students learned that you need to be patient (and also that caramel does not qualify as a crystal); photos/collages by Agustina Pereyra (top left), Antony Becerra (top right), Martina González (bottom left) and Emiliano Velloso (bottom right).

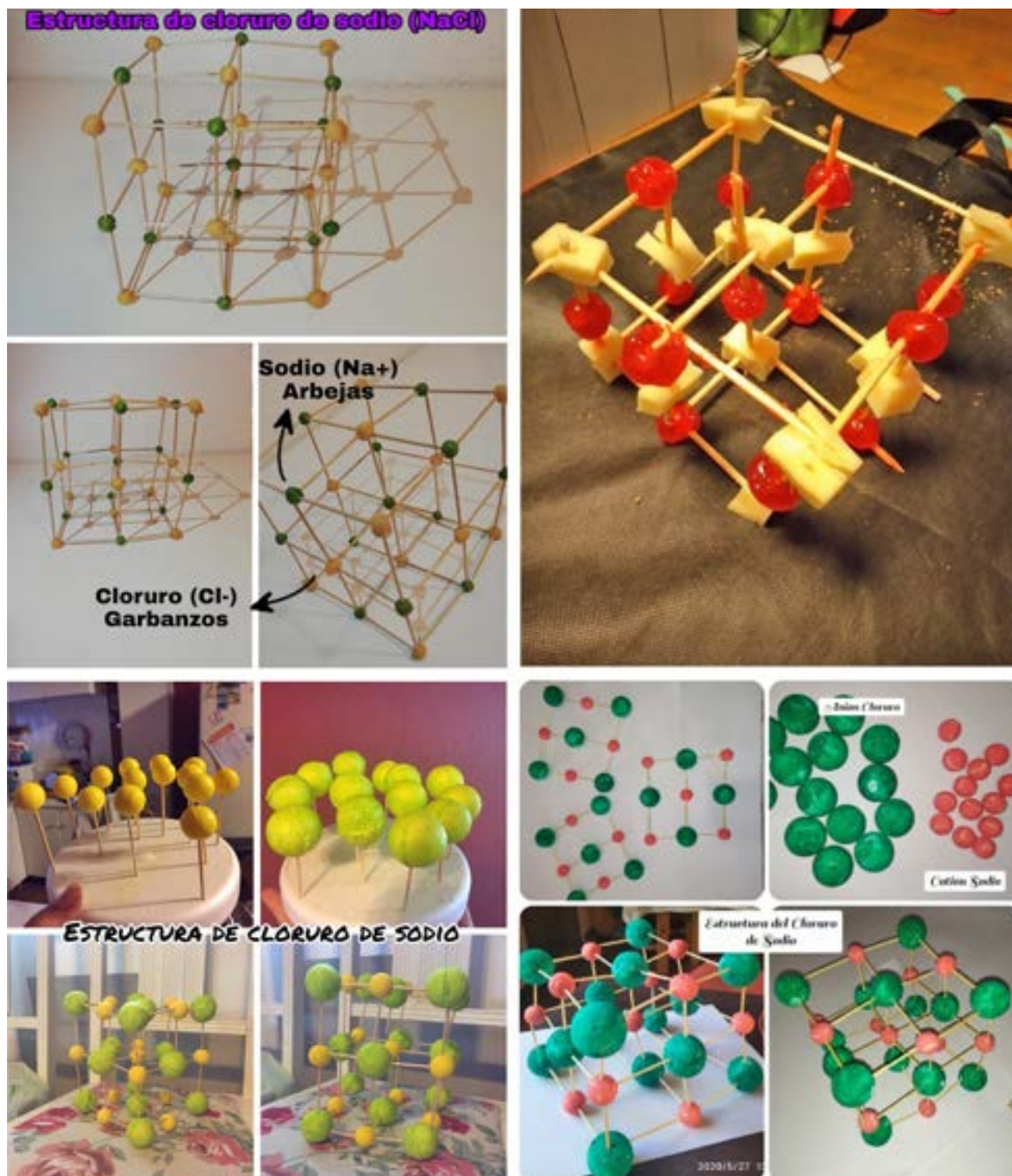
CHCC DESAFÍO #3

En este desafío nos divertimos con un juego de preguntas y respuestas

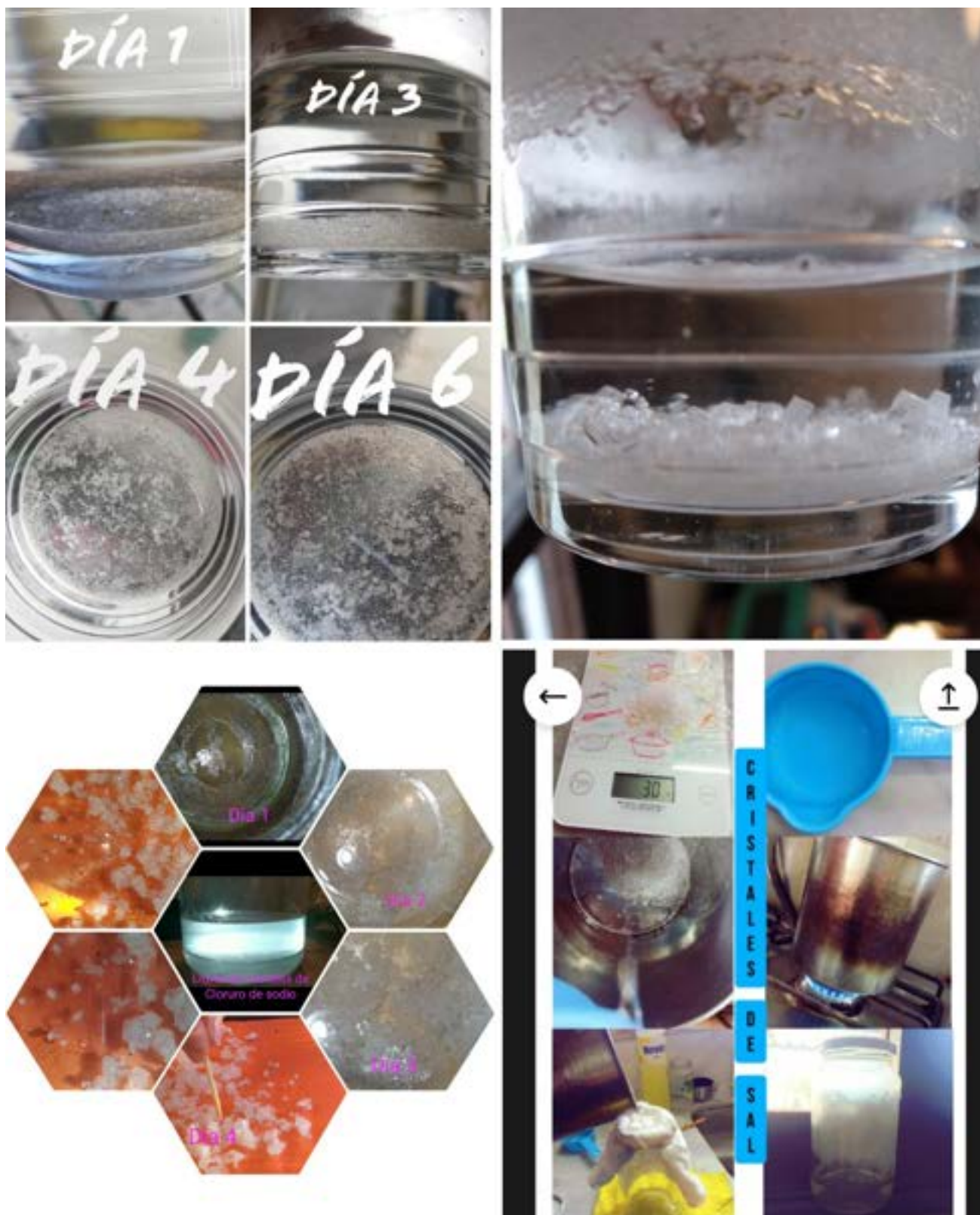
Vos a tener que contestar preguntas relacionadas con cristales. Para responder podés ayudarte buscando información en internet (no te apures, porque no hay tiempo límite entre pregunta y pregunta).

¡Si contestás bien todas las preguntas antes del 18 de mayo podés ganarte hasta 20 puntos!

#3 Ten multiple-choice Kahoot! questions game;



#4 Building a sodium chloride model with elements available at home; photos/collages by Agustina Pereyra (top left), Gabriel Musso (top right), Valentina Villanueva (bottom left) and Martina González (bottom right).



#5 Preparing brine and growing macroscopic salt crystals by slow evaporation, forced precipitation by adding alcohol or salt scales from boiling; photos/collages by Agustina Pereyra (top left), Gabriel Musso (top right), Martina González (bottom left) and Valentina Villanueva (bottom right).

The pictures from each challenge were evaluated by the members of the team (or points in the Q&A game) with 10 points if the pictures were submitted in the proposed time (5 points for late submissions) and 10 points for the aesthetics of the result and the picture, gaining up to 20 points per challenge.

We received more than 50 submissions for the first challenge, close to 100 replies to the Kahoot Q&A challenge and around 20 entries for the challenges that required some manipulation work. The majority of the participants were children in the 8–13 age range, with some teachers encouraging their students to form a couple of groups who submitted the best results within an internal classmates competition. In the end, 16 schoolchildren completed the five challenges. The winners in the first five places received a certificate, a commemorative mug and some CNCC memorabilia as a prize, and the 25 children who completed at least three of the challenges received an electronic certificate.

The event was closed on 20 June after the fifth challenge as all schools re-opened on 1 July.

For the past six years we have continuously run the Uruguay National Crystal Growing Competition. While our seventh edition could not take place, this activity has been extremely rewarding for the organizers, who shared with the participants the uncertainty of these very difficult times. We hope that this report encourages colleagues in other regions to organize activities for schoolchildren, as every minute spent in the organization is paid back with beautiful results and thankful participants, teachers and parents. As long as one child becomes as enthralled by the world of crystallography as we are, we have accomplished our mission for one more year.

We acknowledge the support of Elisa Llambías from Plan Ceibal who assisted us in the implementation of the CREA Group that allowed access to schoolchildren, Facultad de Química – Universidad de la República for financial support and all parents and teachers who put in effort to help the children or students in this Challenge.

Links

- [1] <http://www.cncc.fq.edu.uy/> (in Spanish)
- [2] <https://www.impo.com.uy/bases/decretos/93-2020> (in Spanish)
- [3] <https://www.ceibal.edu.uy/en/institucional>
- [4] http://wiki.laptop.org/go/OLPC_Uruguay
- [5] <http://www.antel.com.uy/empresas/movil/cobertura> (in Spanish)
- [6] https://es.wikipedia.org/wiki/Contenidos_y_Recursos_para_la_Educaci%C3%B3n_y_el_Aprendizaje (in Spanish)
- [7] <https://www.anep.edu.uy/> (in Spanish)
- [8] <http://www.cncc.fq.edu.uy/desafios> (in Spanish)

CRYSTALLOGRAPHY IN AFRICA

On the path of my noble ambition to become an expert crystallographer in Benin: an Italian voyage of discovery

Sidoine A. S. Bonou



Sidoine Bonou at the CIFIESTA Workshop (Naples, Italy) in 2019.

Here, I do not claim to appear or already be considered as an expert crystallographer. Far from it! In fact, this article simply aims to share a series of unforgettable training experiences on my road that will gradually lead me to become, one day, an expert crystallographer following my elders in science, who still make me want to learn more and more every day on the uses of X-ray techniques.

Thanks to the invaluable help and invitation from Sophie Cazalbou and Audrey Tourette of the “Phosphates, Pharmcotechnie et Biomatériaux” research team at the Interuniversity Center for Research and Materials Engineering (CIRIMAT) in Toulouse, France, I spent two months at their facilities in 2016. It was the first time I had come into contact with a powder X-ray diffractometer, and I was trained by Cedric Charvillat, Head of the X-ray Diffraction platform. This short, self-funded internship allowed me to complete my PhD thesis as quickly as possible under the supervision of my professor, Etienne Sagbo. This success opened up many other opportunities for training in crystallography and X-ray techniques by experts at IUCr-UNESCO OpenLabs, schools and workshops. As a compliment on my thesis defense, Professor Cazalbou gave me a copy of *Cristallographie Géométrique* by Nadine Millot. This book was dedicated “to encourage me to become soon an expert crystallographer”. It was a blessing!



Sidoine Bonou as a PhD student with a powder X-ray diffractometer at CIRIMAT (Toulouse, France) in 2016.

A year later, with my work on the “Conversion of *Achatina* snail shell acclimatized in Benin to calcium phosphate for medical and engineering use”, partly carried out with Professor Cazalbou at CIRIMAT, I had the great pleasure of receiving the Best Poster Award at the [Second Pan African Conference on Crystallography](#) (PCCr2) in Accra, Ghana, in 2019. It was the first time I had received a prize at an international meeting with eminent crystallographers coming from all over the world. And to add to the occasion, I received the award from the hands of the IUCr Executive Outreach Officer, Michele Zema, who would go on to play a crucial role in the continuation of my adventure in crystallography. The prize consisted of the IUCr book [A Little Dictionary of Crystallography](#), edited by A. Authier and G. Chapuis. Upon my request, Professor Zema dedicated this book to me, writing “To my friend Sidoine, wishing you a great career in crystallography”.



Sidoine Bonou with his prize for the Best Poster at PCCR2 (Accra, Ghana) in 2019.

At this stage, in my country, the Republic of Benin, great reflections had started and moved in the direction that the scientific future of Benin and all of Africa would be "crystalline" very soon! This is when [LAAAMP \(Lightsources for Africa, the Americas, Asia, Middle East and the Pacific\)](#), founded and coordinated at that time by Sekazi Mtingwa, Michele Zema and Sandro Scandolo (note Marielle Agbahoungbata and Özgül Öztürk were appointed as members of the *LAAAMP* Executive Committee at a later stage), comes into the picture. In fact, following the invitation of *LAAAMP*, Thierry d'Almeida from CEA (France) visited Benin - his home country - and [managed to convince](#) the President and his Cabinet to fund the implementation of a crystallography and tomography facility as part of the Sèmè City innovation center, which became known as [X-TechLab](#). Professor d'Almeida saw in me the character of a young and engaged scientist who was very willing to learn and go further, and wanted me in his working group. I joined the X-TechLab team on the occasion of the organization of the [first training sessions in X-ray crystallography, tomography and mathematical engineering](#), held in Cotonou in May and November 2019, within the framework of the Seme-City-IUCr-UNESCO-LAAAMP OpenLab. The sessions proved very successful and included contributions from eminent professors of international renown.

However, there was a crucial need for me to complete my training in crystallography before taking on the role of Research Coordinator at the X-TechLab, and from 29 August to 11 October 2019, I had the unique opportunity to travel across Italy for various training activities.

Naples

I was first in Naples, from 29 August to 4 September, where I attended the [AIC International Crystallography School "Crystallographic Information Fiesta"](#), organized by Serena Tarantino, Brian McMahon and Michele Zema. This was such a fantastic experience, from both a scientific and a personal point of view. I had the opportunity to meet renowned lecturers and young researchers from around the

globe, fundamental to building my network of contacts in the field. On the occasion of this workshop, the participants produced [two articles](#), one on solving twinned structures and the other a macromolecular structure, which were subsequently published in IUCr Journals. My participation was supported by an IUCr Young Scientist Award, which was highly appreciated as it fully covered my accommodation and subsistence costs.



Michele Zema presenting Sidoine Bonou with the IUCr Young Scientist Award at the CIFiesta School (Naples, Italy).

Bari

With my great enjoyment and increased self-confidence, I learned that my application for an IUCr Young Scientist Award to attend the [EXPO&more Workshop](#) in Bari from 30 September to 3 October had also proved successful. Therefore, I had a three-week gap to fill between the end of the CIFiesta School in Naples and the start of the EXPO&more Workshop in Bari. Professor Zema suggested that I should spend this period in a crystallography lab in Bari, and introduced me to his friends and colleagues Gennaro Ventruti and Emanuela Schingaro, who quickly arranged to have me in their lab for an immersion internship. I learned a lot under their supervision and with the support and availability of their whole team. The training covered several topics, including selection, mounting and centering of single crystals, and data-collection strategies at ambient and high temperatures with a single-crystal diffractometer. Additionally, I received training in the maintenance of detector cooling devices and the programming of data collection on a powder diffractometer. In summary this internship allowed me to learn a bit of everything about powder and single-crystal diffractometers. These skills acquired during such a short period of three weeks deserved to be supplemented by other training.

The EXPO&more Workshop was also very enjoyable and useful as it offered a deep exposure to specific techniques and methods for X-ray powder diffraction.



Left: Angela Altomare presenting Sidoine Bonou with his IUCr Young Scientist Award at the EXPO&more Workshop (Bari, Italy). Right: Sidoine Bonou selecting and mounting single crystals for data collection at the University of Bari, Italy.

Trieste

Like in a scientific adventure where you do not always know where the thirst for knowledge leads, I got the tremendous opportunity forwarded by Professor Mtingwa (*LAAAMP*) to apply for training on the XRD, XRF and XAS beamlines at the Elettra synchrotron in Trieste. So, very soon, it was already time to travel again and move from Bari to the north of Italy. Next stop was Trieste to attend the workshop “Instrumentation for Synchrotron Radiation Experiments” from 7 to 11 October, organized and funded by the International Atomic Energy Agency (IAEA).

I was very elated to interact with eminent scientists at this workshop, which was focused on the preparation, drafting and submission of a proposal for feasible experiments at a synchrotron and a visit to the facilities. Here too, I had very good trainers who impressed me with their teaching methods on X-ray techniques.

In addition to the background acquired in using powder and single-crystal diffractometers in the laboratories of the University of Bari, and to all the theory and practical sessions offered by the workshops in Naples and Bari, this training in advanced light sources at Elettra covered another important aspect, as it focused on the drafting of competitive proposals for an implementation on a synchrotron. Significantly, it was the first time a member of the young team of X-TechLab, *i.e.* I myself, had visited a synchrotron!

My travel experience in Italy for training in crystallography was wonderful because of the succession of opportunities. My commitment is now irreversible!



Sidoine Bonou at the XRF beamline at Elettra (Trieste, Italy), very excited to be on his first visit to a synchrotron.

Acknowledgements

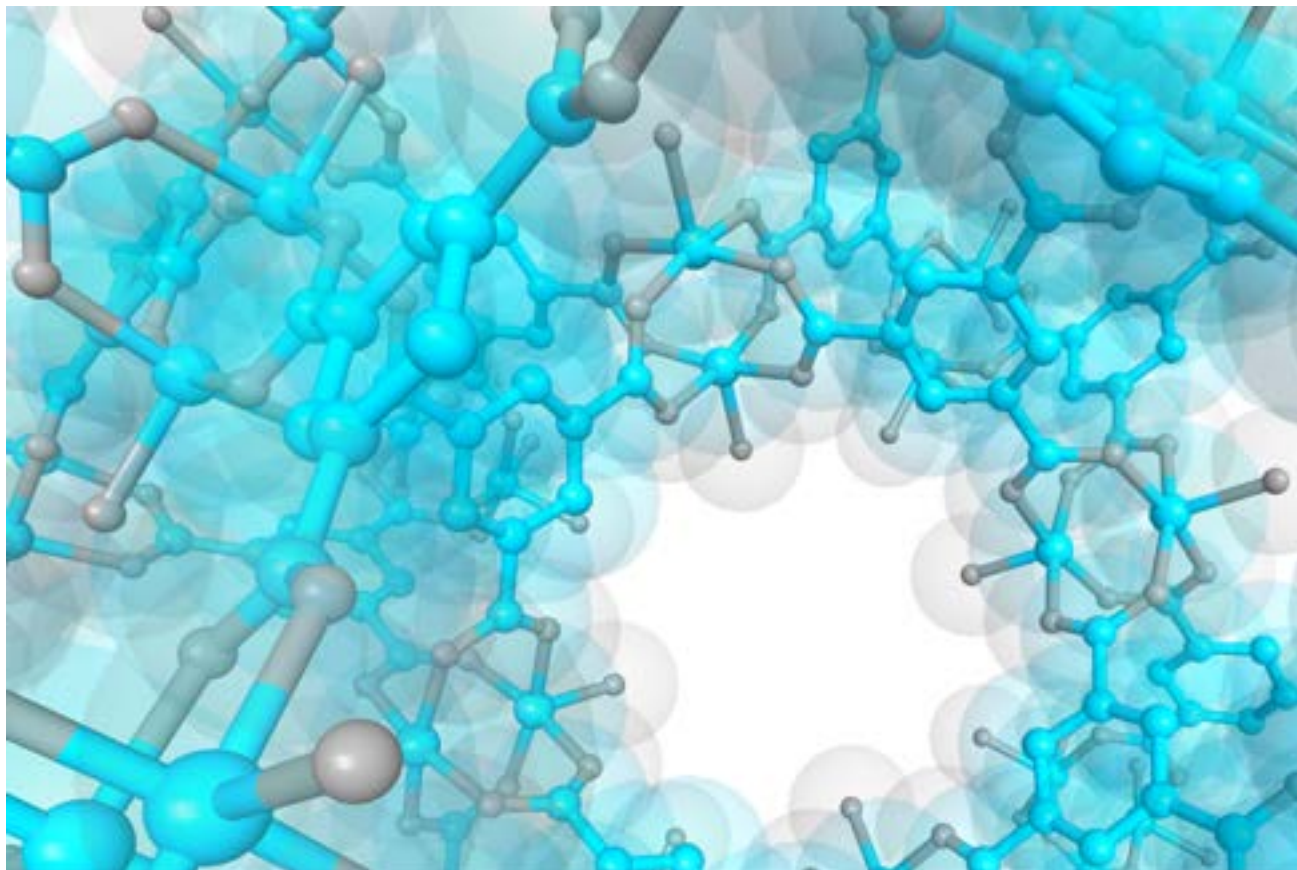
My special thanks go to Audrey Tourette, Sophie Cazalbou, Cedric Charvillat and Etienne Sagbo for my thesis works; to Claude Borna, Head of Agence de Developpement de Sèmè City, to Thierry d'Almeida and Marielle Agbahoungbata, the X-TechLab Project Leader and Coordinator, respectively, and to Michele Zema (IUCr Executive Outreach Officer, Chair of the *LAAAMP* Executive Committee and Chair of the X-TechLab Scientific Committee) for his unwavering support and dynamism. My warm thanks also go to Sekazi Mtingwa (*LAAAMP*), who strongly supports and shares all opportunities to train young scientists at

advanced light sources; Peter Ian Swainson (IAEA) and Hervé Djokpe (Benin Delegate at IAEA); Gennaro Ventruti, Emanuela Schingaro, Ernesto Mesto and Maria Lacalamita (University of Bari) and Anna Moliterni (CNR, Italy) for their fantastic hospitality during my stay in Bari; Serena Tarantino (University of Pavia and CIFIESTA School, Naples); Angela Altomare (EXPO&more Workshop) and her team; Alessandro Migliori (XRF beamline), Guiliiana Aquilanti (XAS beamline) and Jasper Plaiser (XRD beamline) at Elettra Sincrotrone Trieste; and all supervisors who contributed to my training during this special travel period.

MEETING REPORT (IUCR SUPPORTED)

First International School on Advanced Porous Materials

Valentina ColomboSimona GalliJorge A. R. Navarro



The [First International School on Advanced Porous Materials](#) (MOFSchool2019), which took place from 17 to 21 June 2019 at Villa del Grumello, Como, Italy, as part of the events patronized by the Lake Como School on Advanced Studies, was attended by 78 participants - 54 students, 10 teachers, the representatives of 2 commercial sponsors and the Organizing Committee members. The cultural and scientific exchange certainly benefited from the presence of a vast number of foreign attendees, coming from up to 21 different countries of the 5 continents. The school, dedicated to an audience of young students, neophytes to the chemistry of porous metallorganic materials, focused on the synthesis and characterization of these materials, as well as on a number of representative applications (e.g. CO₂ capture, water capture, volatile organic compounds capture and separation). To this aim, several front lectures and one hands-on session were organized. In more detail, the school covered the following topics:

- Synthesis and post-synthesis methods; reticular chemistry; selective capture of greenhouse gases or water from air (Omar Yaghi). Professor Yaghi also gave an informal evening lecture on personal anecdotes connected with the scientific discoveries realized in his laboratories over the past 20 years.
- Advanced characterization methods: spectroscopies (Silvia Bordiga); single-crystal X-ray diffraction (Felipe Gándara); powder *in situ* X-ray diffraction (Valentina Colombo); X-ray absorption (Kirill Lomachenko).

- Topological description and hands-on session with the software *TOPOS* (Davide Proserpio and Vladislav Blatov).
- Structural flexibility and defects introduction (Roland Fischer).
- Role of unsaturated metals as active sites and their characterization; use of structural flexibility for the capture/release of industrially relevant gases and the cooperative adsorption of CO₂ and other strategic gases (Jeffrey Long).
- Integration of porous materials within circuits for applications in electronics (Rob Ameloot).

The young participants were given the opportunity to present their research during one flash-presentation session and two poster-presentation sessions. Six prizes were offered for the best poster and flash presentations by the IUCr, Berkeley Global Science Institute, *Chemical Society Reviews* and *CrystEngComm* and awarded to six young participants.

The school benefited from a number of different financial contributions. The IUCr fund supported the accommodation or travel expenses of three students, namely Avena Maia Renata (Universidade Federal do Rio de Janeiro, Brazil), Jung Minji (Gyeongnam National University of Science and Technology, Korea) and Rajak Richa (Indian Institute of Technology Indore, India).

MEETING REPORT (IUCR SUPPORTED)

Gordon Research Seminar on Crystal Growth and Assembly

Elias Nakouzi



The 2019 Gordon Research Seminar on Crystal Growth and Assembly, which took place at the Southern New Hampshire University in Manchester, NH, USA, from 22 to 23 June 2019, presented a unique forum for graduate students, postdocs and other scientists to engage and discuss exciting topics related to crystallography. The meeting focused on topics ranging from the fundamentals of nucleation and crystal growth to the formation of thin films, hierarchical structures, biominerals and beyond. In addition to these engaging scientific discussions, the Gordon Research Seminar (GRS) provided an excellent opportunity for professional development and networking across our research community. The meeting preceded a five-day Gordon Research Conference (GRC) on the same topic that was also attended by professors, industry professionals and program managers.

The meeting organizers consisted of one male and one female, the line-up of speakers consisted of four male and four female speakers, and similarly the discussion leaders for the sessions were four males and four females. To add to the international flavor of the meeting, the represented countries among these 18 scientists included Russia, Mexico, Poland, China, USA, The Netherlands, Israel, UK, The Philippines, India, Lebanon and Cyprus.

The meeting was kicked off with a welcome note from the organizers Elias Nakouzi and Yael Tsarfati, who thanked the attendees and noted that the attendance (77 scientists) had doubled from the previous

version of this meeting in 2017. We also thanked the sponsors, including the IUCr, for their role in supporting this increased attendance.

The Keynote lecture was given by Bart Kahr (NYU), who presented a historical perspective on the research field, then journeyed from basic crystallography theory to state-of-the-art results through a simple question: “Why are crystals straight?”.

The Mentorship Component was a lecture by Dave Blake (NASA Ames) titled “Reflections on Building a Spacecraft Instrument: The Development of the CheMin XRD/XRF”. Dave was the PI of the CheMin instrument that accomplished a seminal milestone in the field of crystallography, namely crystallography on another planet aboard the Mars Research Lab (Curiosity Rover). The talk revisited a career-long journey of failure and ultimately success and included a lively Q&A session on the science and – perhaps more importantly – advice for early-career researchers.

The meeting included a vibrant poster session as well as a social time where colleagues shared drinks, snacks and conversations. These events were very successful in breaking the ice in preparation for the subsequent GRC. The credit for that success goes to the GRS/GRC meeting structure.

There are several collaborations that we know of that have resulted from this meeting. Also, multiple participants have since moved to new positions within the same research field as part of their next career steps. We hence anticipate that the appetite for the next version of the meeting in 2021 will be healthy, hopefully fuelled by a return to normalcy in a post-COVID world.

MEETING REPORT (IUCR SUPPORTED)

24th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXIV 2019)

Chunhua Tony Hu Michael D. Ward Bart Kahr



Yael Tsarfati, winner of the IUCr Journals Poster Prize at ICCOSS XXIV 2019.

Since its inception in Brookhaven (USA) in 1968, the International Conference on the Chemistry of the Organic Solid State (ICCOSS) has become the premier forum for discussing groundbreaking research on the chemistry and physics of organic materials. We were proud to host the 24th conference, [ICCOSS XXIV 2019](#), at New York University, NY, USA, from 16 to 21 July 2019. The program showcased frontier research from a slate of international experts, with curated sessions that represent the cutting edge of organic solid-state chemistry. The conference had many opportunities for informal conversations as well as some special sessions that addressed societal and career issues. The scientific program for ICCOSS XXIV included invited and contributed lectures, as well as poster sessions. In addition, an exhibition of scientific instruments, electronic resources and books took place. The conference schedule consisted of eight technical sessions: (1) Crystals that Move, (2) Crystals in Computers, (3) Crystals that Grow, (4) Crystals in Devices, (5) Crystals in Nature and Medicine, (6) Crystals and Light, (7) Crystals in 2D and (8) Crystals with Holes. These topics represent the forefront of research in organic solid-state chemistry, from dynamics in crystals to machine learning for crystal structure prediction to crystals in medicine.

There were 53 oral presentations in total, of which 17 were contributed from female speakers (32%) and 36 from male speakers (68%). One of them come from Africa, 12 from Asia, 1 from Australia, 13 from Europe, 25 from North America, and 1 from South America.

The conference hosted 162 registered attendees, of which 60 were female (37%) and 102 male (63%). Three of them come from Africa, 39 from Asia, 1 from Australia, 26 from Europe, 90 from North America, and 3 from South America.



Group photo of attendees.

IUCr Young Scientist Awards

Three young scientists were selected to receive financial support from the IUCr to attend ICCOSS XXIV:

María Cecilia Dávila, an undergraduate student at the Universidad de Los Andes, Venezuela, working in the research group of Graciela Díaz de Delgado. Her research focuses on crystallography of pharmaceutical polymorphs. She presented a poster titled “Metal Derivatives of an API with Incommensurate Modulated Structures”.

Qiang Zhu, an assistant professor at the University of Nevada, Las Vegas, NV, USA. His research focuses on the development of first-principle structure predictions based on evolutionary algorithms and their applications. He gave an oral presentation titled “Crystal Structure Prediction: From Code Development to Applications”.

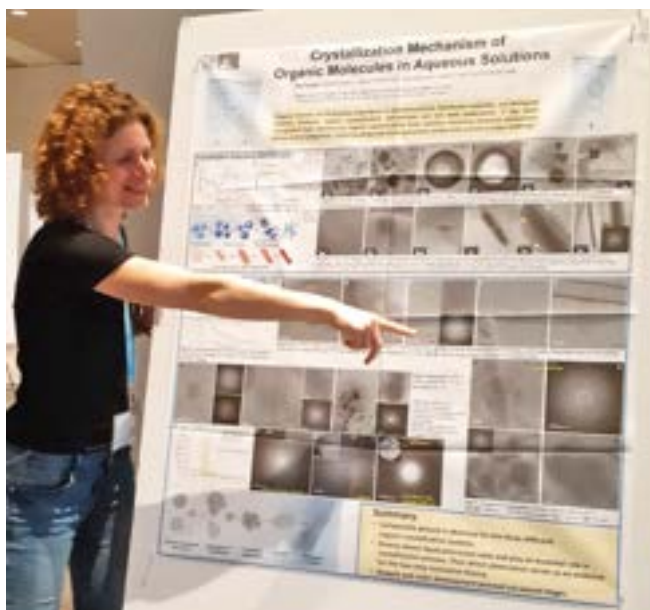
Noa Marom, an assistant professor at Carnegie Mellon University, Pittsburgh, PA, USA. Her research focuses on quantum mechanical simulations combined with machine learning and optimization algorithms to computationally design materials with desired properties for various applications. She delivered an oral talk on “Property-Based Genetic Algorithm Optimization of Molecular Crystals for High Carrier Mobility”.



(Left photo) María with Bruce Foxman (left) and Ian Duncan Williams (right) in the poster session, and (right photo) Qiang Zhu presenting his research.

IUCr Journals Poster Prize

Yael Tsarfati (Weizmann Institute of Science, Israel) won the IUCr Journals Poster Prize. She received a voucher for the second edition of Joel Bernstein's book *Polymorphism in Molecular Crystals*. She is working on the understanding of crystallization of organic molecules in the group of Boris Rybtchinski. Her winning poster's title was "The Mechanism of Non-Classical Organic Crystallization".



Yael Tsarfati talking about her poster.

Summary

The success of ICCOSS XXIV relied on many factors, of which one of the most important was the financial support to the young scientists attending the conference. The conference organizers are very grateful to the many organizations generously providing support to these brilliant young scientists.

MEETING REPORT (IUCR SUPPORTED)

Latin American Crystallographic Association activities in 2019

José Antonio Henao Miguel Delgado Graciela C. Díaz de Delgado



II LACA School 2019 (top) and IV LACA Meeting 2019.

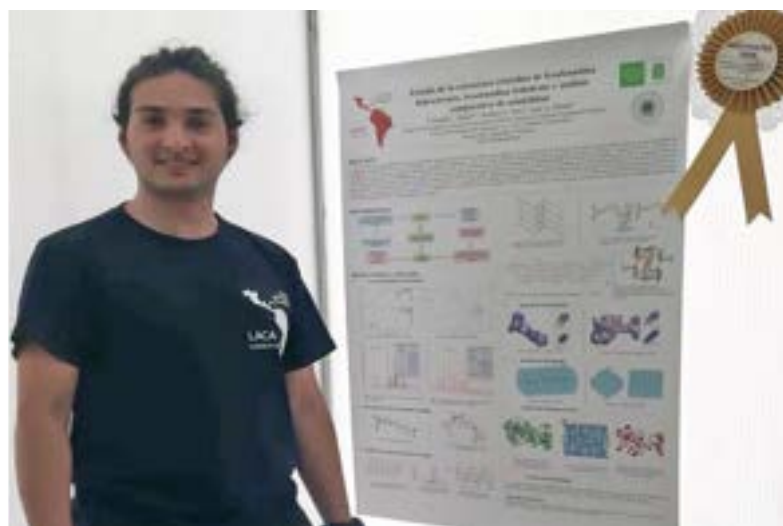
The Latin American Crystallographic Association (LACA) had two main events in 2019. The II LACA School took place 1–6 October and the IV LACA Meeting 7–10 October at Universidad Industrial de Santander (UIS), Bucaramanga, Colombia. José Antonio Henao (UIS) was the Chair of the organizing committee.

The program of the II LACA School included lectures and demonstrations on single-crystal and powder diffraction techniques and was taught by 11 international and 3 Colombian instructors. A total of 75 young researchers and students from Bolivia, Brazil, Chile, Colombia, Costa Rica, Ecuador, Mexico, Peru and Venezuela attended the school; 28 of them were awarded scholarships through IUCr funding and 17 received scholarships from the International Centre for Diffraction Data (ICDD). The female-to-male ratio for the participants was 47:53. In addition to financial support, the IUCr provided online access to *International Tables for Crystallography* during the school. The Cambridge Crystallographic Data Centre (CCDC) provided licences for 30 days to the Cambridge Structural Database and the ICDD to the PDF-4 databases.



Recipients of IUCr Young Scientist Awards at II LACA School.

The IV LACA meeting included plenary lectures delivered by IUCr President Sven Lidin (Sweden), Abel Moreno (Mexico), Silvia Cuffini (Brazil) and Iris Torriani (Brazil), who received special recognition for her long-standing scientific career and for her work for the Latin American crystallographic community. Attendees were from Argentina, Bolivia, Brazil, Chile, Colombia, Costa Rica, Ecuador, Germany, Italy, Mexico, Peru, Sweden, Uruguay, the USA and Venezuela with a 40:60 female:male ratio. A total of 35 young scientists received travel and subsistence support from the IUCr; the IUCr also supported the attendance of two Visiting Professors, James Kaduk (USA) and Serena Tarantino (Italy). The meeting included 12 semi-plenaries, oral presentations, posters and a commercial exhibit. From the two poster sessions, eight posters presented by students were selected for prizes awarded by LACA, IUCr Journals, ICDD's *Powder Diffraction* journal, the CCDC, *Journal of Chemical Crystallography*, *CrystEngComm* and *Crystal Growth & Design*.



Cristian Camilo Rojas Sepúlveda (UIS), winner of the IUCr Journals poster prize at IV LACA Meeting.

The Colombian Crystallography Society met for the first time during the meeting. At the assembly, the need to strengthen collaboration between laboratories and to activate the adherence of Colombia to the IUCr were discussed and approved. A committee composed of representatives from UIS, Universidad Nacional de Colombia, Universidad del Valle, Universidad de Los Andes and the Colombian Geological Service was set up to take the necessary steps for Colombia to apply for membership of the IUCr during the next General Assembly in Prague in 2021.



The Colombian Crystallographic Society with Graciela Díaz de Delgado, IUCr Representative on LACA, on the far right.

At the LACA Assembly, the report on the activities carried out in 2018–2019 was presented by LACA President José Reyes-Gasga (Mexico), as well as Professor Torriani. Professor Moreno presented a proposal to host the 2026 IUCr Congress and General Assembly in Mexico, and the LACA Assembly approved support for a bid from the Mexican Crystallography Society (SMCr) to host this event. The LACA Assembly discussed the planning of the 2021 and 2022 meetings, with Costa Rica and Uruguay as possible sites for the V and VI LACA meetings. As the IUCr Congress and General Assembly has been postponed until 2021, the LACA meetings will also be postponed to 2022 and 2023.

MEETING REPORT (IUCR SUPPORTED)

16th Conference of the Asian Crystallographic Association (AsCA2019)

Edward Tiekink



The acrobatic Lion Dance at the Conference Banquet.

The 16th Conference of the [Asian Crystallographic Association](#) (AsCA) returned to Singapore 27 years after the first AsCA meeting, which was organised by the late Koh Lip Lin [Department of Chemistry, National University of Singapore (NUS)]. The venue for AsCA2019 was UTown at NUS and commenced with four almost fully subscribed [pre-Conference Workshops](#) (CCP4-Protein Crystallography, CSD, Olex2 and TOPAS) held over 15–17 December and conducted by renowned world experts. This set the tone for the formal Scientific Programme, which started with the Opening Ceremony on the afternoon of 18 December, officially opened by the President of AsCA, Jenny Martin.



Official Opening: Jenny Martin, President of AsCA 2016-2019.

The Opening Ceremony was followed immediately by the first of three Plenary lectures delivered by Myunghee Kim, with Susumu Kitagawa and Donglin Jiang presenting on subsequent days. These outstanding contributions were complemented by six Keynote lectures presented by Ruchi Anand, Robert Dinnebier, Alison J. Edwards, Masako Kato, Zhi-Jie James Liu and Chilla Malla Reddy (<https://asca2019.org/plenary-and-keynote-speakers/>). In developing the Scientific Programme, a key underlying principle was to ensure a broad and fair representation of the AsCA crystallographic community at all levels of the Conference. This was greatly facilitated by the **Flash Presentation** innovation whereby nearly 50 younger participants from a broad range of laboratories had the opportunity to present highlights of their Poster Presentations in a one-slide/three-minute format. The Flash Presentations made up 3 of a total of 24 microsymposia encompassing the three broad themes of Macromolecular Crystallography, Chemical Crystallography, and Materials and Applications. One of these microsymposia was dedicated to lectures by the six successful **Rising Star Awardees**, who were presented with their prizes at the Conference Banquet, which featured an acrobatic Lion Dance and an occasional address by a former IUCr President, Gautam Desiraju.



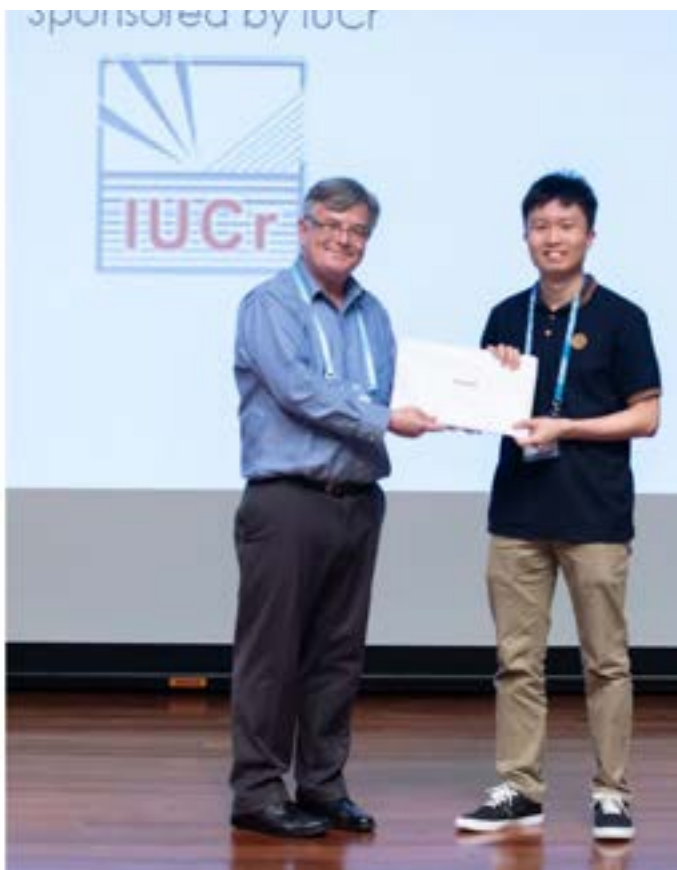
Awards Ceremony at the Conference Banquet for the Rising Stars. L-r: Raghavender Medishetty, Rumpa Pal, Palash Sanphui, Gautam Desiraju, Deepti Sharma, Ryo Suzuki and Haruki Sugiyama.

In terms of numbers, the conference attracted about 485 registrants from 28 countries with a gender breakdown of 32% female and 68% male. The largest delegations were from Japan (93), India (68), Korea (64), People's Republic of China (46) and, the hosts, Singapore (55). Active participation in the Conference, including all lecture presentations and chairing/co-chairing sessions (over 300 roles) saw a female:male ratio of 32:68. The participant numbers were augmented by about 40 exhibitors, which resulted in a "full house". The Conference Organisers are extremely grateful to the many **exhibitors and sponsors** of AsCA2019 and we wish to highlight here our four Platinum Sponsors: Bruker, Crest, Dectris

and Rigaku. The sponsorship gained from so many diverse and generous organisations enabled the establishment of many categories of prizes and awards. Through the generous support of the IUCr, there were 24 [IUCr Young Scientist Awardees](#), many of whom were able to present their excellent work as Oral Presentations during the meeting. The Awards Ceremony in the closing session of AsCA2019 saw awards to all successful presenters and was quite a busy occasion.



Awards Ceremony in the Closing Session.



AsCA2019 Programme Chair Edward Tiekink presents the IUCr Journals Poster Prizes to (left) Shailabh Tewari (Indian Institute of Technology Delhi, India), Chemical Crystallography category, and Takeshi Matsukawa (Ibaraki University, Japan), Materials & Applications category. Jing Yuan How (not pictured, La Trobe University, Australia) won in the Macromolecular Crystallography category.

In any conference, much of the effort is divested to various committees *etc.* but there is always the one key go-to person. The entire AsCA community is extremely grateful for the wonderful efforts of JJ Vittal, the Chairman of the Local Organising Committee, for making AsCA2019 such a memorable occasion involving so much of our diverse Asian crystallographic community and beyond.



Local Organising Committee Chair, JJ Vittal.

All are welcome to visit the [AsCA2019 home page](#) for more details and the [photograph gallery](#) for (downloadable) images.

MEETING REPORT (IUCR SUPPORTED)

70th Annual Meeting of the American Crystallographic Association (vACA2020): “Training the Next Generation”

Nozomi AndoCarla Slebodnick



Coronavirus illustration by David S. Goodsell, RCSB Protein Data Bank; doi: [10.2210/rcsb_pdb/goodsell-gallery-019](https://doi.org/10.2210/rcsb_pdb/goodsell-gallery-019).

We are pleased to report that the [70th Annual Meeting of the American Crystallographic Association](#) was successfully transitioned under these unprecedented times from an in-person San Diego, CA, USA meeting to a virtual meeting (vACA2020). The scientific program was held from 2 to 7 August 2020, with workshops and other events held the weeks before and after the scientific program. The meeting, which had a theme of “Training the Next Generation,” attracted 605 attendees, of which 293 were students or postdocs.

With the remarkable work of many volunteers and organizers, the vACA2020 was able to preserve many elements of an on-site meeting, despite being conducted over *Zoom*. The meeting kicked off with a three-day Small Angle Scattering Workshop, which made use of the virtual format to provide hands-on training to many more participants than is normally possible. The scientific sessions included plenary lectures from 2020 ACA Award winners as well as parallel sessions with invited and contributed talks (many of them given live), followed by live Q&A. Special events included the plenary COVID-19 session, which drew a wide audience (despite Hurricane Isaias affecting internet connectivity for some), and an

interactive poster session highlighting the work of many young scientists. The meeting was capped with a two-day Cryo-EM Workshop, which featured lectures and lively panel discussions.

The scientific sessions represented many topics in biology, chemistry, geosciences, materials science, communications, and education and outreach. In the last category, a notable highlight was a presentation on molecular storytelling by David Goodsell. Scientific topics went beyond traditional single-crystal and powder X-ray diffraction techniques to include next-generation methods and facilities such as cryo-EM, micro-electron diffraction and advanced capabilities at national synchrotron and neutron sources. The conference also sought to empower the next generation by including sessions that were a balance between scientific research findings and technique know-how. By minimizing the cost to students and postdocs and making the workshops free, young scientists were able to take full advantage of conference opportunities, including giving nearly 50% of the oral/poster presentations and receiving practical training through the four workshops.



A meeting highlight was the plenary session, which was sponsored by MiTeGen: *Structural Contributions to SARS-CoV-2 and the COVID-19 Pandemic*. This session outlined the remarkable contribution that structural scientists have made toward understanding the SARS-CoV-2 virus and potential routes to therapeutics and vaccines. Stephen Burley (Rutgers/RCSB PDB) opened the session by outlining how the PDB has curated and overseen the distribution of over 300 SARS-CoV-2-related structures. Andrzej Joachimiak (ANL) focused on the high-throughput structure determination of nonstructural coronavirus proteins toward understanding the binding mechanism and development drug targets. Nir London (Weizmann Institute) continued the discussion of drug targets by sharing how structural results are being “crowdsourced” to help with the design, characterization and modeling of new drug targets. Joanne Lemieux (University of Alberta, Edmonton) presented on the feline coronavirus drug GC376 and its mechanism of inhibition of the main protease of SARS-CoV-2 to block virus replication. Ian Wilson (Scripps) talked about the study of the antibody receptor binding domain to the spike protein toward vaccine development. The session concluded with Jason McLellan (UT Austin) who discussed the structural changes that must occur in the spike protein for virus entry into cells and the possible mechanism of disrupting these changes.

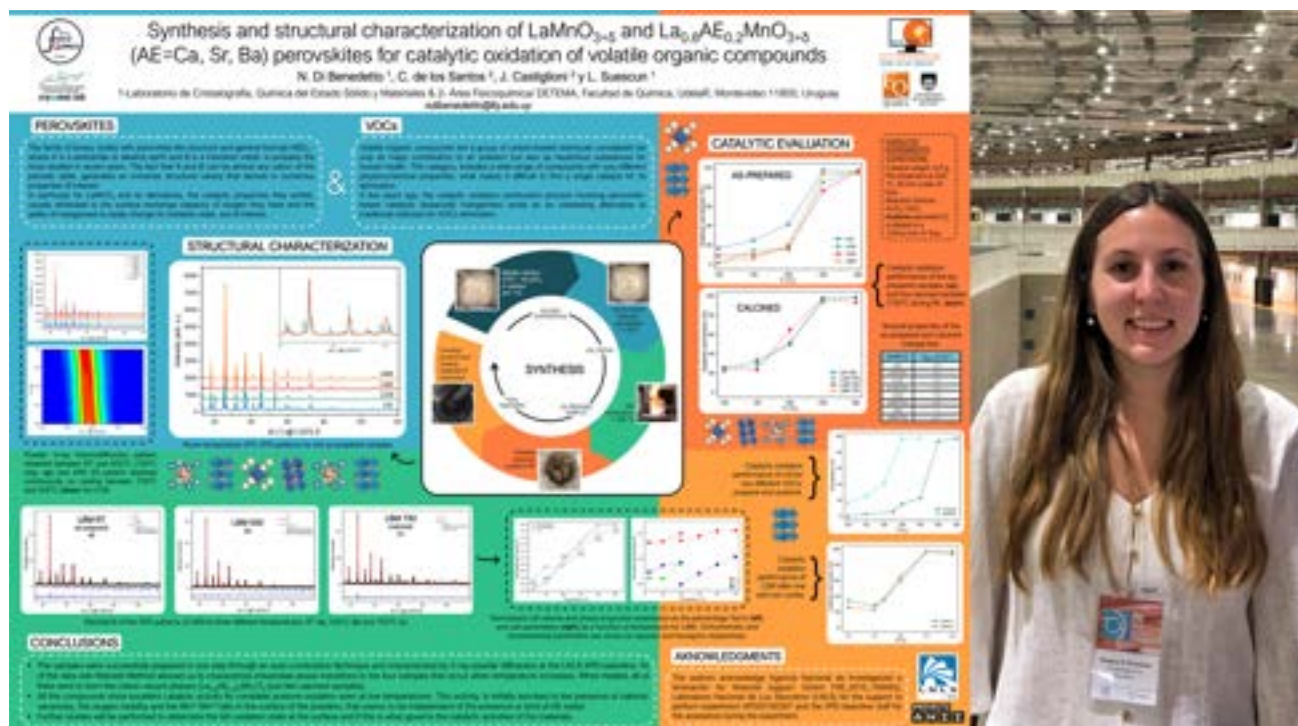
Plenary lectures were given by the 2020 ACA Award recipients:

- Margaret C. Etter Early Career Award: Nozomi Ando (Cornell), "Protein Allostery."
- David G. Rognlie Award: James Holton (UCSF/LBNL/SLAC), "If I had a Trillion Dollars."
- A. L. Patterson Award: Václav Petříček (Czech Academy of Sciences), "Don't be Afraid of Modulated Structures."
- Elizabeth A. Wood Science Writing Award: Brenda MacArthur (The Alan Alda Center for Communicating Science at Stony Brook), "Creating Connections: An Introduction to the Alda Method[®]."

Four virtual workshops were offered in association with the meeting. The virtual program had the benefit of allowing us to avoid schedule overlap enabling registrants to attend as many workshops as they wanted giving a total of 635 workshop registrants. Workshops included the following:

- Applications of Small Angle Scattering to Structural Biology: An Introduction
- Introduction to Hydroxyl Radical Foot-printing Methods for Structural Analysis of Proteins and Complexes
- Introduction to Diffuse Scattering Analysis from Single Crystal Neutron Diffraction
- Fundamentals of Single Particle Cryo-EM

The ACA also congratulates our [poster awardees](#) who are too numerous to mention individually.

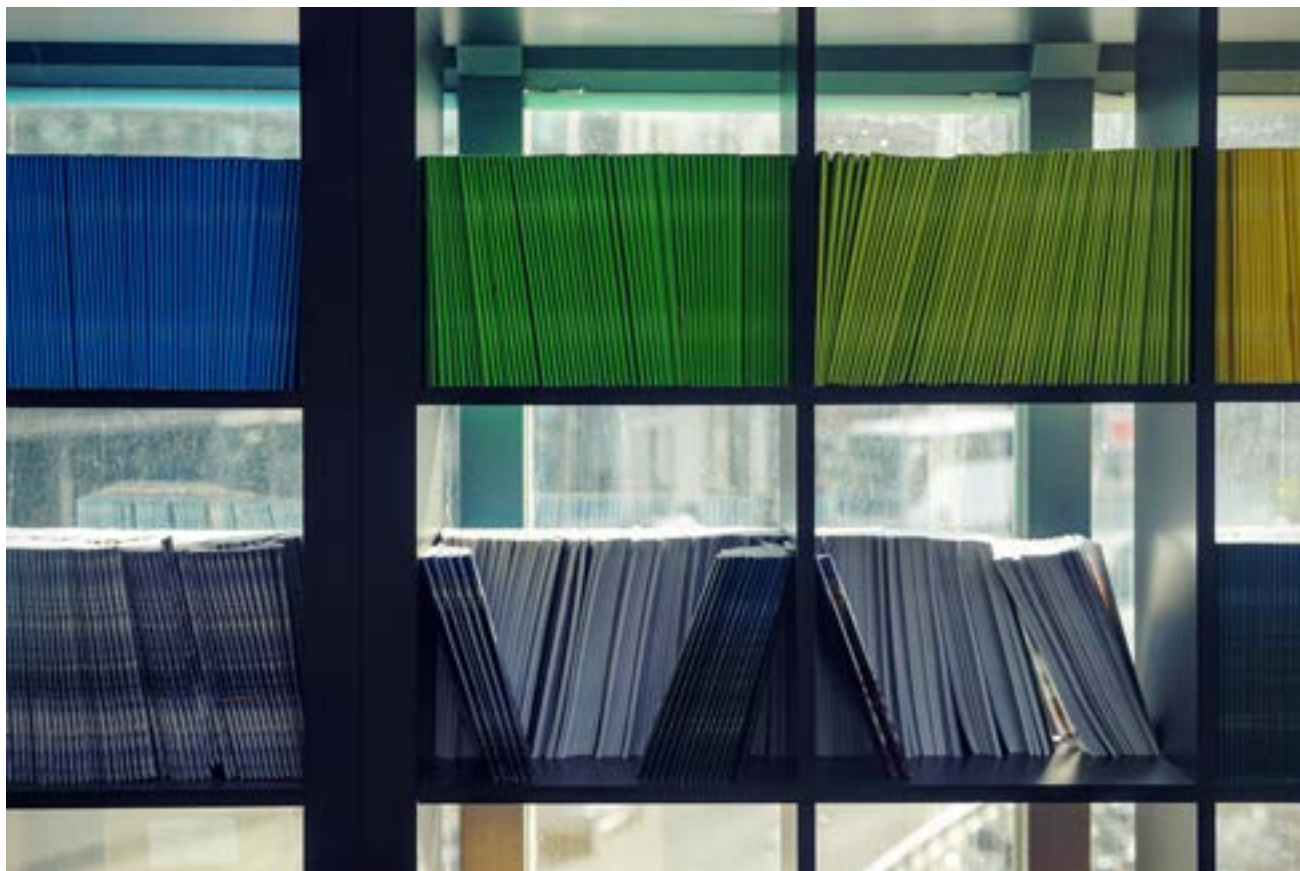


The IUCr Poster Prize was won by Natasha Di Benedetto (Universidad de la República, Montevideo, Uruguay) for her presentation "Synthesis and structural characterization of $\text{LaMnO}_{3-\delta}$ and $\text{La}_{0.8}\text{AE}_{0.2}\text{MnO}_{3-\delta}$ (AE = Ca, Sr, Ba) perovskites for catalytic oxidation of volatile organic compounds".

We would like to thank our sponsors including MiTeGen, Rigaku, Bruker, AIP, ThermoFisher, *Structural Dynamics*, Dectris, SerCAT, *Crystal Growth and Design*, *Inorganic Chemistry*, Stanford-SLAC Cryo-EM Center, sptlabtech, anatrace and IUCr Journals.

NOTICE

Back issues of Acta Crystallographica available to a good home



The IUCr has learned that Dr Geoffrey Pitt, a crystallographer who trained in Dorothy Hodgkin's lab in Oxford, UK, after WW2, has four bound volumes of *Acta Crystallographica* dating from 1948 to 1951 (Volumes 1 to 4) available free of charge to a good home. Collection from the M3/North Hampshire area required. Please contact support@iucr.org if interested.

Subsequent note: these back issues have now found a home and are no longer available.

HISTORY OF CRYSTALLOGRAPHY

Rosalind Franklin British coin

Mike Glazer



Recently, the Royal Mint in the UK produced a splendid 50 pence coin in honour of Dr Rosalind Franklin and her famous Photograph 51 of DNA. As a result, there was a lot of discussion in the Twittersphere about this coin. Initially, some of us, including myself (!), thought that this looked more like a modern X-ray rotation diffraction image typically from a protein crystal *i.e.* with its high density of spots. Surely we would expect to see the X-shaped diffraction pattern typical from a fibre. However, we were, in fact, misled by this regular pattern of spots in the image. Basically we knew too much diffraction! If you look carefully, and most significantly if the coin is tilted, one can then make out more obviously the original image with its dark cross typical of a helical structure – clever!

So, I recently ordered a gift pack from the Royal Mint and received a nice little booklet together with the coin. Here, I read that the designer was David Knapton, a member of the Royal Mint's graphic design team. In his own words: "A straight representation of Photograph 51 wouldn't have worked on a coin, so I decided to reflect the printing techniques of the era. To restore Franklin's rightful role, it was important to include her name. Adding an A to a third column to line up with the last letters of Rosalind and Franklin to spell DNA felt like a small "penny drop" moment. I can only imagine how Franklin felt when she made her breakthrough discovery."

"Printing techniques of the era" refers to the pointillist style for newspapers, even today, and not to forget the paintings of the pointillists such as Seurat. The accompanying booklet from the Royal Mint gives a brief resume about Rosalind, mentioning that the photograph was taken by her student Mr Raymond Gosling at King's College, London, in May 1952. It also notes that Professor Maurice Wilkins,

having shown the image to Dr James Watson, had provided the final clue that Watson and Crick needed to model the double helix structure of DNA, their second attempt, having been corrected by Rosalind in their first attempt (paraphrasing: "phosphates not on the inside, which would have repelled, but on the outside").

If you want to order a gift pack, you can do this from [here](#).

Addendum

You may be wondering why the 50 pence coin in the UK is seven-sided. I used to tell people that this meant that it was not possible to place these coins together on a table without leaving gaps, thus making it easier to pick up with fingers. However, while possibly being true, this is not the reason. I am continually learning new things. This particular shape can be shown mathematically to form an equilateral-curve heptagon, or Reuleaux polygon, a curve of constant width, meaning that the diameter is constant across any bisection. This allows the coin to be used in a vending or sorting machine without it being dropped in a particular orientation. And, oh yes, a bag of them is handy for crystallography tutorials to illustrate that you cannot completely tile a surface with them, as with regular pentagons.

Note

It is worth noting that a remarkably similar photograph was obtained a year earlier by Elwyn Beighton working in Bill Astbury's laboratory in Leeds (UK) (see [here](#)) but whose significance was not appreciated by Astbury at the time. I recommend the book *The Man in the Monkeynut Coat: William Astbury and the Forgotten Road to the Double-Helix* by Kersten T. Hall for the full story.

HISTORY OF CRYSTALLOGRAPHY

Walter Friedrich unplugged: his 1963 interview in East Berlin

Peter J. HeaneyMelanie Kaliwoda



Figure 1. Walter Friedrich in 1962 (from [German Wikipedia](#)).

Prefatory remarks

Walter Friedrich (1883–1968; Fig. 1) was the first person to build a device that successfully achieved diffraction of X-rays by a crystal, and he was the first to observe the diffraction pattern produced. This epochal accomplishment simultaneously demonstrated the wave-like nature of X-ray radiation and the translational symmetry that defines crystallinity. Had Friedrich performed this study today, he might have been named a co-winner of the Nobel Prize. Instead, Friedrich's status as a postdoctoral researcher on temporary loan from Arnold Sommerfeld to a Privatdozent, Max von Laue, situated Friedrich on the lower rungs of the German academic hierarchy. Consequently, Laue was named the sole recipient of the Nobel Prize in Physics in 1914, and Friedrich's contributions seem eclipsed by the likes of the Braggs *père et fils*, Paul Ewald, Peter Debye and Laue himself. As evidence, the English language *Wikipedia* includes an entry for *Friedrich Walter*, an Austrian hockey player of the 1940s, but nothing for Walter Friedrich, who instead is memorialized only in the German *Wikipedia*.

Laue was always generous in recognizing Friedrich and his other junior collaborator, Paul Knipping, Sommerfeld's graduate student at the time. Laue gave Friedrich and Knipping senior authorship of seminal papers on X-ray interference (Friedrich *et al.*, 1912, 1913) and sole authorship of two others (Friedrich, 1913a,b), he acknowledged them in his Nobel lecture, and he offered them a share of his prize

winnings. Nevertheless, Friedrich's important place in history has been obscured by additional factors: two years following the diffraction experiments, Friedrich left solid-state physics to focus on biological radiography, a field in which he made pioneering discoveries but remained outside the orbit of the physics community. Moreover, in 1947 Friedrich accepted an appointment at the University of Marburg, which was located within the Soviet sector of Berlin, and he thus became a citizen of the German Democratic Republic, further limiting his activities with western scientists. Finally, Friedrich was a modest man who habitually downplayed the importance of his creative contributions relative to those of Laue.

As the historical record shows, however, early X-ray diffraction theorists – including Laue and the Braggs – were mired in deep misapprehensions. Even if one is not persuaded by all elements in Forman's (1969) attempt to debunk the mythology surrounding the birth of X-ray diffraction, it is clear that the premonitions of Laue and William Lawrence Bragg were well-divorced from physical reality. Laue proposed that stimulation of a crystal by an X-ray beam would induce heavy atoms to fluoresce characteristic X-rays, whose interactions with an *electron lattice*¹ would yield a diffraction pattern. That is why Friedrich's first experiments led to the placement of photographic plates to the sides rather than behind the crystal – of triclinic chalcantite ($\text{Cu}_2\text{SO}_4 \cdot 5\text{H}_2\text{O}$), hardly the first mineral an omniscient crystallographer would choose to authenticate the diffraction process. Conversely, W. L. Bragg's (1912) intuition that X-rays reflect from planes of atoms remains a spectacularly useful but erroneous metaphor. Paradoxically, in his first effort to demonstrate the mirroring of X-rays by atomic planes within a muscovite wafer, he placed a photographic plate *behind* the crystal, not in the reflective Bragg-Brentano geometry so familiar to us today. Experimentation was the only path that could lead through the fog of theory towards an approximation of truth, and Friedrich's proficiency with X-ray instrumentation gained from his six years as a doctoral student with Röntgen was crucial to the success of this transformative research.

Friedrich recounted the story of the discovery in several published documents, including a decadal anniversary paper in *Naturwissenschaften* (Friedrich, 1922) and a reminiscence in the same journal 27 years later (Friedrich, 1949) – both in German. His impressions were not included among the personal remembrances in the semicentennial volume edited by Paul Ewald (Ewald, 1962). Thomas Kuhn and colleagues spearheaded an effort in the 1960s to 'find and preserve primary source materials for the study of the history of quantum physics' (Kuhn *et al.*, 1967), and these archives include approximately 100 interviews, available online through the American Institute of Physics. Perhaps to correct the omission in Ewald (1962), Gustav Hertz, Théo Kahan and John L. Heilbron travelled to East Berlin to interview Walter Friedrich in May 1963. Hertz (1887–1975) was a postdoctoral assistant to Heinrich Rubens at the University of Berlin in 1912; he was collaborating with James Franck on inelastic collisions of electrons in gases, for which he won the 1915 Nobel Prize in Physics. At the time of the interview, he was *ordinarius* professor at the University of Leipzig and chairman of the Physical Society of the GDR. Théodore Kahan (1904–1984) was a French physicist who authored two dozen books on radioactivity and quantum physics. John Heilbron (born 1934) was working on his doctoral studies with Thomas Kuhn at the time of this interview. He is a Professor of History and Vice-Chancellor emeritus at UC Berkeley, and he has won many awards for his research into the history of science, including the George Sarton Medal in 1993. He is a member of the Royal Swedish Academy of Sciences.

Both Knipping and von Laue had passed away at the time of the interview – Knipping was riding a motorcycle that was hit by a car in 1935 and Laue was driving a car that was hit by a motorcyclist in 1960. Friedrich was, therefore, able to speak without fear of ruffling feathers, but there are no salacious revelations in this 1963 interview. Indeed, those familiar with the many outstanding reviews of the X-ray diffraction revolution (e.g. Ewald, 1962, 1969; Eckert, 2012; Authier, 2013) will recognize much of what Friedrich has to say. Nevertheless, the interview offers genuine rewards: one senses his keen intelligence, wry humor and self-deprecating modesty. Despite his obvious affection for Laue, Friedrich emphasizes that these discoveries were not predetermined by theorists. In addition, those of us who have advocated for a greater appreciation for the role that mineralogists played in developing notions of

ordered atomicity will appreciate the affectionate description of Paul von Groth, the professor of mineralogy at the University of Munich (Heaney, 2020). As a physicist in Munich in the early 1900s, Friedrich resided at one epicenter of quantum mechanics, and his research intersected with many of the luminaries who set the stage for the birth of modern physics, including Röntgen, Sommerfeld and von Laue. These reminiscences bring these characters back to life.

Acknowledgements

This interview was conducted as part of the Archives for History of Quantum Physics (AHQP) project, and we thank Professor Heilbron for sharing his memories of the AHQP with us. The original recording was remastered onto 10" reels and sent to the American Philosophical Society. We gratefully acknowledge the American Institute of Physics (AIP) for allowing the reproduction of this full interview, designated as: Friedrich, Walter on 1963 May 15: in German. Niels Bohr Library & Archives, American Institute of Physics. One Physics Ellipse, College Park, MD 20740. Original document, transcription and translation are available [online](#). PJH acknowledges the support of a travel grant to Munich by Penn State Global Programs and NSF Grant EAR-1925903. The authors thank Professor A. M. Glazer for his editorial handling of this contribution.

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Interview with W. Friedrich

Conducted by: Gustav Hertz, John L. Heilbron and Théo Kahan.

Place: East Berlin, East Germany.

Date: 15 May 1963.

Tape No. 69, Side 1(a).

WF: I was involved with X-rays already as a high school student, and I still have an invoice from the magistrate of my hometown for 8 X-rays, 28 Deutschmarks. I have a receipt that says: 'W. Friedrich, high-school student.' That was in 1902. I was a student in Geneva, and I actually wanted to be a musician there. I had always played the violin, and I studied with a famous violinist.² But my father asked "Well, how are you going to be a great violinist?" I said "I don't know yet." He said "There are people in your class who play better than you!" I admitted "Yes, there are." "So, you won't be a great violinist."

Then I resignedly returned to my old love of physics and continued my studies in Munich with Röntgen (Fig. 2).³ I was with Röntgen for six years for my studies and as an assistant. I also completed a dissertation on X-rays with Röntgen. After finishing my doctorate, I was an assistant with Arnold Sommerfeld⁴ for three years. It was something like 1909 to 1913; I don't remember the exact period. There I also met Professor Ewald,⁵ who I believe is now in America,⁶ and also Professor von Laue,⁷ who came from Berlin at the time and became a Privatdozent in Munich to continue working with Sommerfeld there. Ewald was working on a doctoral thesis with Sommerfeld on the subject: 'The optical behavior of electro-magnetic waves when passing through an electron lattice.' He had some difficulties in performing the mathematical derivations and asked Max Laue for assistance, and Laue helped him with it. At this time, Laue came up with the idea: if the X-rays have a wavelength as short as was assumed based on diffraction experiments with narrow slits, then they would have to give X-ray interference patterns when passing through an electron lattice, through a crystal. This was discussed for about a quarter of a year in the cafés, as was the custom in Munich at the time.



Figure 2. Wilhelm Conrad Röntgen in 1900 (from [Wikimedia](#)).

TK: Who was there?

WF: Ewald and Laue.

TK: You were there too?

WF: No, I wasn't there at all. I heard about it from their later conversations. I had a job studying X-rays with Sommerfeld. I had an X-ray machine, at that time, one of the most intense and powerful X-ray machines, and I had to do some work on particular properties of X-rays and Planck's quantum theory, okay? Sommerfeld had certain ideas about Brehmsstrahlung radiation, whether or not it was controlled by quantum processes *etc.* I was there shortly after these discussions. And we talked about it (X-ray interference) for a long time, and the strange thing is that none of the people who were at the meetings, including Röntgen and Sommerfeld – also Mie⁸ when we were skiing and Starke⁹ (and Wald and Jort)¹⁰ – these were the main people at the time: they didn't think it would work. And I almost have forgotten Willy Wien¹¹ from Würzburg, even though he had worked with X-rays at his Institute.

And it was kind of forbidden to do an experiment. "This is not possible; it is superfluous; the thermal vibrations will prevent it (X-ray interference) from happening." No, people have forgotten, but as we now know, there were statistical problems too. There was only a certain probability that the locations and positions of atoms according to the space lattice were regular, and it seemed like a longshot, you know, that we would observe interference; as we later proved, we needed long-exposure periods. And we talked about it, and I said to Laue, "Well, let's do it in the back (of the lab), let's do it in the evening," all right? [Chuckles]. And since, as I said, during the day I was busy with my work with Sommerfeld, my seminar assignments – you know what it is like in an institute – we brought in another student, Paul Knipping.¹² He had just finished his PhD work and was writing up and had some time.

We built a very simple apparatus, a diaphragm through which X-rays 1 mm or 2 mm in diameter passed, a large locked lead box containing a plate holder and a crystal holder, which was just a tripod (Fig. 3). Since we had misconceptions about the nature of these interferences, we first thought – and we should have known better, by the way – that it was the characteristic radiation of the crystal that triggered the interference. That is why we examined copper sulfate, because we thought we were generating the characteristic radiation of copper. Today, we know that this radiation is not at all coherent – just as fluorescent radiation is not optically coherent. As such, no interference could have come from the copper radiation.

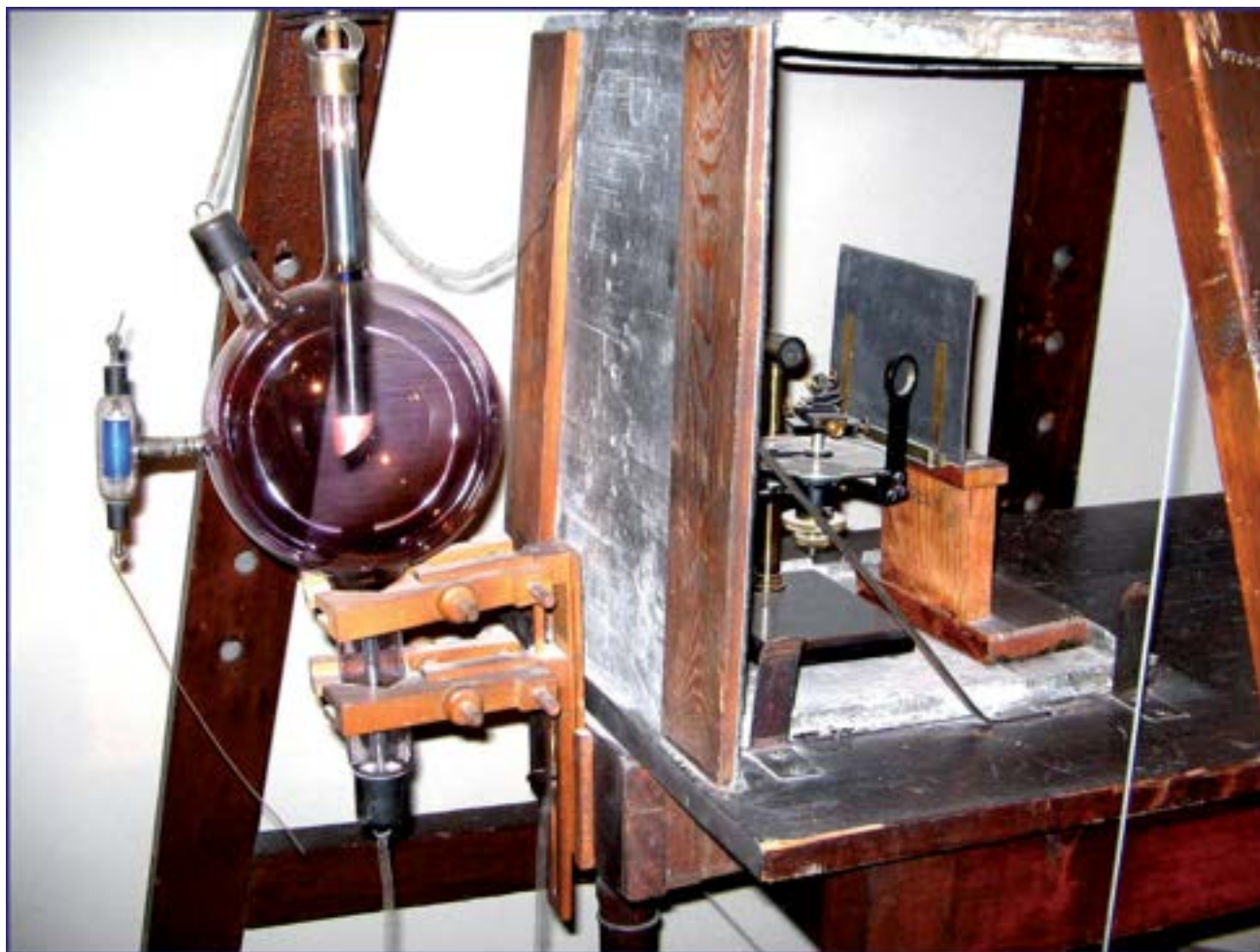


Figure 3. Friedrich's experimental apparatus for the first X-ray diffraction experiment. Copyright: Deutsches Museum in Munich.

Anyway, because I knew about X-rays, I thought: "Well, let's just irradiate the crystal for ten hours." So we irradiated for ten hours. At that time, we were still using the gas-containing tubes that had to be regenerated. We used a palladium tube, which is quite permeable to hydrogen, and the tubes had to be regenerated over and over again. We waited for ten hours. And in the evening it was around 11 pm that I took the plate out and put it in the developer tray, and then suddenly a black blob emerged, a black spot from the unscattered X-rays. In addition, there were ring-shaped patterns that were quite irregular, of course, because firstly, the mineral belongs to an irregular crystal system, okay, and also because it was not oriented. And next to these patterns, there was the shadow of a pitcher [Laughter].

TK: A pitcher?

WF: A mug, a Munich mug, a beer mug (Fig. 4). And how did that come about? Because the non-directional radiation, the scattered radiation, cast a shadow of a so-called screw-ring. The crystal was inserted into this screw-ring. This shadow appeared on the plate as a body, short and wide, and the handle on the ring also stuck out. Now, of course, you can imagine my great surprise. I went to Knipping in the morning, and we went to Laue and then finally to our boss and showed it to him.



Figure 4. The first diffraction pattern of chalcantite, taken by Friedrich and Knipping and signed by Laue, in the shape of a Munich beer mug.

TK: Your boss was Sommerfeld?

WF: Yes, Sommerfeld. We also showed it to Röntgen *etc.* and they were quite surprised. Of course, we immediately tackled other things – first of all, a regular crystal, and considerations of characteristic radiation led us to sphalerite (a variety of ZnS).

TK: For what reason?

WF: Because we thought the characteristic radiation of zinc was the radiation that would yield interference patterns. We had a jeweller cut a beautiful plate from a sphalerite crystal and grind it perpendicular to the fourfold symmetry axis, and we mounted it in the apparatus. We now had a goniometer as part of it *etc.* The instrument was now much more complicated and finished. Also, different sections of sphalerite, cut in different directions, were examined. We took another picture with a long exposure time. And behold, the beautiful fourfold symmetry was there (Fig. 5).

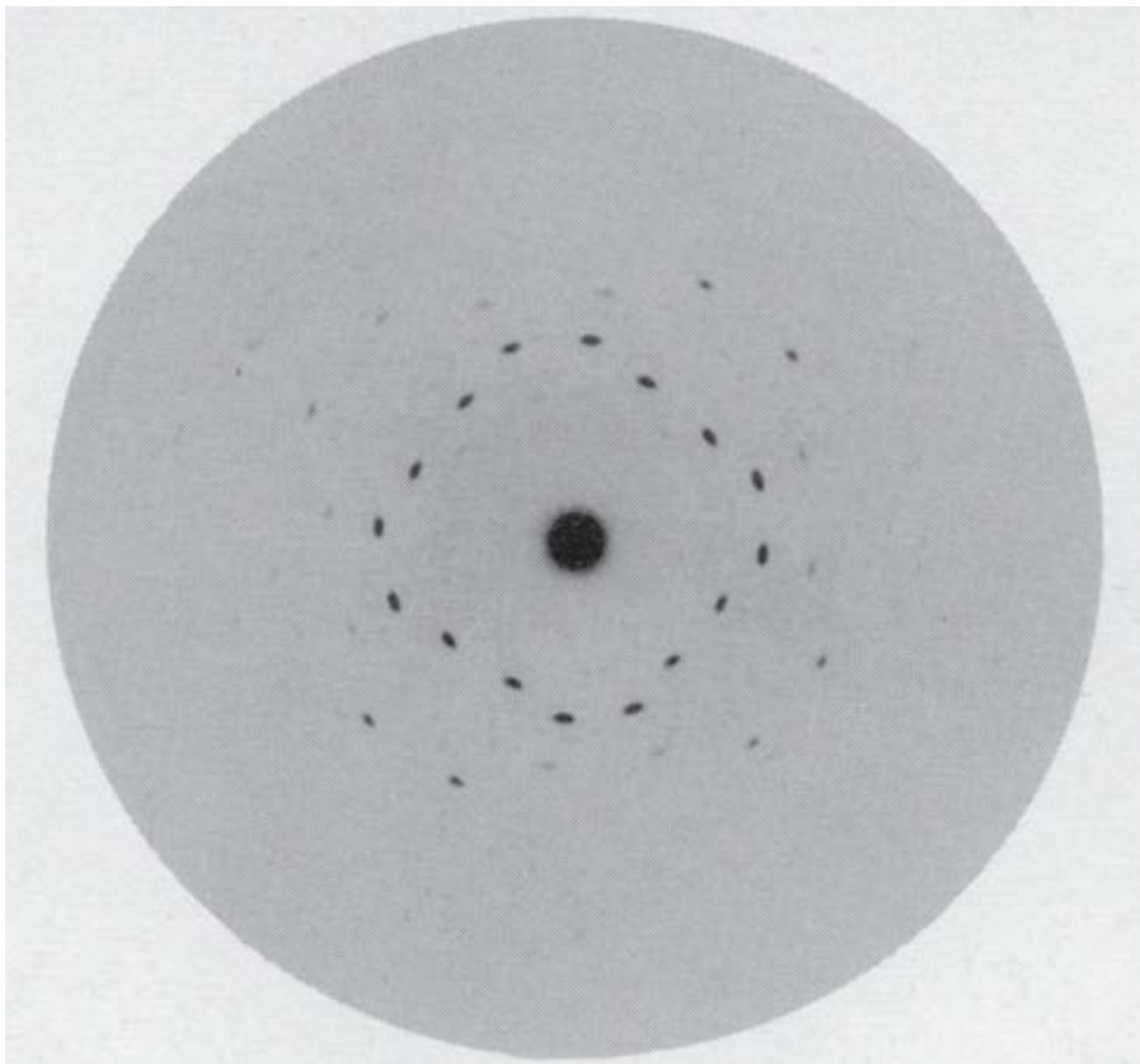


Figure 5. The first published X-ray diffraction pattern along the fourfold axis of sphalerite (Friedrich *et al.*, 1913a). Open-access article from *Annalen der Physik*.

Now you can imagine the great joy! But here was the situation: Max Laue had intuited the phenomenon but did not yet grasp the theory. That's why we had no idea what it would look like! We expected it would be a blurry thing, and we had set up plates in all directions and were now surprised that suddenly there were very sharp interference spots.

Now Laue sat down straight away and tried to do the right thing as an optical physicist according to the classic theory of optics. That was the difference between him and Bragg,¹³ isn't it true? He (Laue) developed the theory from the old theoretical formulas about interference, these empirical formulas, and in this way, he was now able to derive equations, which then contributed to the interpretation of this interference phenomenon. He found that there were different wavelengths involved. He did not specify the wavelengths directly but invoked a parameter, where a is the lattice constant. In any case, this was the presumption made by Laue. Later it was said that we planned it in this order, that his theory emerged, and then the experiments were performed. In reality, the experiments came first and then the theory followed. That is a mistake, which may give rise to some misinterpretations of the entire history. That's how it was.

Now it was easy. Next, the threefold symmetry axis was examined, then the twofold symmetry axis, then isomorphic crystals and also regular crystals. Then the question of thermal vibrations came up. We just made things less complicated – no cooling etc. of the crystal – by using a diamond crystal. At that time, the theory of specific heat told us that diamond is one of those solids that, at room temperature, has the same properties that other bodies exhibit at low temperatures. So we got a diamond plate from Röntgen, which he had obtained from Ereus (the Ginsberg Company) from Hanau.¹⁴ The experiments with this diamond plate showed that the interference was much more pronounced, not only in the direction of the beam, but also in the direction away from the beam, so that, you know, it became apparent that thermal vibrations have an effect, but that this influence is not so great because solid matter is essentially static.¹⁵ And there's only a change in intensity –

[Two voices obscure dialog.]

– the change in intensity revealed the appearance of new interference spots that would not otherwise have occurred during normal exposure times. And so it is, on such occasions, you can discover something else when you are not looking for it. For example, I wanted to take a picture, or rather, we wanted to take a picture. The height of the crystal was a bit high in the goniometer because of the optical setting, and it had to be lowered so that the X-rays could pass through it. The crystal was glued to the mount with adhesive wax, and the X-rays passed through the adhesive wax instead of through the crystal, which was not intended. And what did you see on the photograph? Rings, a ring, right?

And we thought about it for a long time and finally came to the conclusion that these were either (direct images of) the large molecules that composed the adhesive wax or, more likely, that the wax is a liquid crystal; we would not call the wax a solid crystal. A physicist in Karlsruhe, you know him better than I, (Otto) Lehmann,¹⁶ described these crystals. And we now recognize that wax is completely disordered, and as a result, the interference pattern exhibited rotational symmetry. This is the same thing that Debye¹⁷ later achieved with his powder patterns, where the crystals adopt all possible orientations, all possible directions. Consequently, the probability that interference occurs in a certain direction is represented by rotational symmetry, *i.e.* a ring. Well, that was published a bit later.

TK: May I ask a question? The length of time from the – from the moment that Laue's suspicions began –

WF: Half a year.

TK: – and the first photograph? Half a year?

WF: Nobody believed that!

GH: Half a year, too strange.

WF: Of course, nobody believed that! We went skiing. They had a rough idea in, let's say something like 1911, and then in 1912, the pictures were taken. But behind the scenes, you know. It's like, if you think about it, this nice idea wouldn't have been confirmed at all if I didn't have an X-ray machine, and if I hadn't worked with X-rays, and if we hadn't done it behind the scenes, it would have gone nowhere.

TK: Undercover work! [Laughter]

WF: Then it would have been discussed, over and over, "Well, you see, it's written here who did it."

GH: What did Laue think about it? Did he think that it made no sense?

WF: No. Laue thought it had to work. From the start, he didn't accept the objections concerning thermal vibrations because of his enthusiasm for the idea. That was the main reason that we thought "For God's sake, a lot of people have been skeptical of things and later it was done, so let's do it, we have everything here!" The X-ray machine was here, my experience in working with X-rays and so on. As a result, it all went very well. It was done in a few weeks.

And above all, I always emphasize that it was an extremely nice collaboration, you know? I encountered some difficulties later.¹⁸ It is true that Professor von Laue was awarded the Nobel Prize for it. He shared it with us; of course, Stockholm did not recognize us,¹⁹ but he gave us credit. I received letters from Stark,²⁰ you know: "Don't put up with that, etc." Yes, yes, yes. I have always taken the stance that I wouldn't have done it without the idea! I made the discovery, but I wouldn't have done it on my own. As a result, there was never any kind of animosity between us. On the contrary, we were friends until his death (Fig. 6).



Figure 6. Max von Laue (from [Wikipedia](#)).

TK: You didn't have any difficulty with Knipping, did you?

WF: No, no.

TK: I was told a great story that he became very angry and destroyed the equipment. Did such a thing happen?

WF: Why would he? He later passed his exam and was here at A.E.G.²¹ He worked here, and then he came to Darmstadt, where he established a small institute. He was hit by a car and didn't live long. It's strange, isn't it, that all the people who worked there were involved in an accident. Sommerfeld was hit by a car, Laue was hit by a car, or at least had a car accident. The only thing missing was that I... [Chuckle]

JH [in English]: Can Professor Friedrich tell us a bit about the history of the quantum during his time in Munich? How Sommerfeld got interested in the quantum and so on?

TK [Translating]: Colleague Heilbron would like to know if you can tell us something about the quantum hypothesis in Munich, about the changing views on quantum theory.

WF: We know, of course, in Sommerfeld's Institute that Sommerfeld was very busy with quantum theory, and, as I said earlier, the experimental work that I started in his Institute was directed towards quantum theory, just as my PhD thesis was. My doctoral thesis was focused on measuring the azimuthal intensity distribution of X-rays. [Illustrating with his hands.] So when the cathode rays come from here, and this is the anode, right, there is a particular distribution, which is called the azimuthal distribution. And this distribution depends on the speed of the cathode rays. This is not a symmetrical distribution, but it goes in the direction of the cathode rays, so to speak, where the maximum is. And if not, if this were an asymmetrical distribution, it would have to be assumed. And that's what Sommerfeld had already started thinking about, and he wanted to have this verified by a new study, where you could separate and then measure this intensity distribution so that one would have a clean image of the Bremsstrahlung radiation.

GH: When was the law for the short-wave limit actually found?

WF: It was found later using X-ray spectroscopy by the Braggs, wasn't it? Röntgen, for example, didn't understand much of Laue's theory, you know, because Röntgen was an experimental physicist, and when he saw the integration of such and such, you can imagine that a theory developed purely on the basis of theoretical physics was difficult for him. But when he heard Sir William Bragg's perspective on the theory, akin to how the colors from thin films appear, how the coloration on the surface of a drop of oil is caused, that was immediately clear to him. That the crystal is built up like a book from layers, and when the X-rays hit the surface, a few are reflected from the top layer, and then a few from a little bit further down, giving rise to certain path differences and interference effects: that was much more vivid for him. And now, based on their theory, the Braggs built a real X-ray spectrograph, and they found the diffraction limit. That limit, of course, has been a pillar of quantum theory, you know, because it was related to v^2 of the electron.

GH: I think the gentleman also wanted to know whether you remember the initial discussion about the Bohr model, how it became accepted, whether you remember something about this among the Munich circle of scientists. It is always very difficult to remember this afterwards.

WF: Yes, yes, it is always very difficult. It was clear, of course, that Bohr's work, in particular, was very well received by us, that there was a lot of discussion in the colloquia as well, especially in the Sommerfeld seminar – a seminar that was more like a colloquium because it was not so much about teaching material, but about new views and new work etc. There was a lot of discussion about it, but as much as I can remember, things were a bit – well, how can I say – well, now I am supposed to find the right expression – so insufficiently theoretically founded, that it was a kind of fantasy, first of all, a fantasy structure that, in his mind, was perhaps the answer to the question that this model posed, but it wasn't really properly founded. In this regard, Sommerfeld was much too precise a theoretical physicist, who was likely wondering: 'How is this actually theoretically sound?' But it was initially only a model, one perspective before the matter was further substantiated.

TK: When did you leave Munich, please?

WF: I left Munich for a strange reason because I then degenerated into medicine.

TK: Which year?

WF: 1914.

TK: You had already left Munich.

WF: I left Munich with the permission of Sommerfeld, initially for a year, because I had a lot of contact with medical professionals, and I heard from them that when using physical forms of energy, like X-rays, light rays etc. they actually knew nothing about the basis of the effect, even the physical basics, the biological basics. And then I went to Freiburg. There at the women's clinic was a gynecologist, a gynecologist whose name was (Bernhard) Krönig,²² and he was very interested in this matter. And if you considered it, you know, so what do the people who use X-rays actually know of the effects, of the properties of X-rays? An engineer from the factory from which you bought your X-ray machine came and instructed you a bit. But if you know how to work scientifically and you delved into it, you could see a new field of biophysics that was ready to blossom. So we then together wrote a book on the biological and physical-biological basis of radiation treatment. These were all our own experiments, where all the properties and laws were to be found. And that has actually been the basis of bio-physics (Fig. 7).



Figure 7. Bronze bust of Walter Friedrich cast in 1964 by Maria Shockel-Rostowskaja, located on the biomedical Campus Berlin-Buch GmbH (from [German Wikipedia](#)).

Later in Germany, a former industrialist, Dessauer,²³ championed this field; he was a great diplomat. Do you know what he did? I wouldn't have had that idea. He was a member of the Reichstag in the Zentrum Party and, at the same time, a member of the city council of Frankfurt. I knew him personally for a long time, and we were very closely acquainted with each other, and because he pondered a lot of scientific questions, he said: "Frankfurt must have a university!" He founded a university!

GH: Oh, he did?

WF: He did so with the help of the Reichstag, okay, where he was a Zentrum delegate, and also with the help of the magistrate. They founded a university in Frankfurt, and he was called a Professor of medical physics. That was how he went from factory director to Professor [Chuckle]. But then he had an assistant, you all know him, Rajewsky, (Boris) Rajewsky,²⁴ who is now in Frankfurt, was an assistant to Dessauer.

TK: May I ask another question? Who attended the Sommerfeld seminar, the Sommerfeld colloquium? Who were the physicists? Were there experimental physicists there?

WF: Yes, experimental physicists were also there, although very few, mostly because experimental physicists lacked the mathematical tools. Back then, it was not the way it is now. Incidentally, Sommerfeld was the first to push his students into theoretical physics, because before that was Leo Graetz²⁵ and – what were their names – oh God, they treated theoretical physics with all the variables in the old way, wrote formulas that not only covered the whole blackboard but needed several rows of blackboards. The first one who actually introduced modern theories of mathematical analysis was Sommerfeld.

TK: Debye was already there?

WF: Debye was my predecessor as an assistant.

GH: When I was a student with Sommerfeld, Debye was an assistant.

WF: Yes, yes, he was my predecessor, and Debye came to Aachen at the time. He was already habilitated and came to Aachen, and I became the successor and then came Ewald. Ewald was in Göttingen and then for a while in England. Then he came back to Berlin and Munich and then went back to England. My colleague was Lenz, the theoretical physicist from Hamburg, Wilhelm Lenz,²⁶ who mainly worked in electrodynamics as a major subject. But Sommerfeld's first lectures, the very first simple, descriptive working methods that he taught the students so that they could employ them for theorizing – vector analysis, for example – were first delivered in Munich by Sommerfeld. And of course, it was problems such as those in analytical mechanics, where everything became very clear from the use of vectors etc.

JH [in English]: It's most interesting that von Laue first heard of the crystal model from Ewald, and I wonder whether the lattice model was better known to the experimentalists?...

GH: The gentleman means whether experimental physicists were actually aware of the concept of a crystal lattice before the discovery?²⁷

WF: No, no. We had a friend, old [Paul Heinrich Ritter] von Groth,²⁸ who was the mineralogist, the crystallographer. The physicists always liked him because he was an extremely nice and friendly man, and his field was always used as an exam subject. The physicists were examined in mathematics, theoretical physics, experimental physics and another subject. You could take chemistry or something else, and we always took mineralogy, because when we went to the collection of crystals and minerals, there on Neuhauser Strasse in Munich, you met old Groth. He said to you: "Well, young friend, you are also interested in these things," and then he handed his book over to you, and when he heard that you took his subject, mineralogy, as a minor, he said: "Well, you don't know that much about mineralogy. If

you are a little bit interested in crystals and individual classes, I will ask you about that" [Chuckle]. And that's why Groth himself was our advisor afterwards in the choice of the other crystals that we examined.

TK: He was a professor of mineralogy at the university?

WF: At the University of Munich, yes.

[Gustav Hertz leaves.]

TK: I want to ask a bibliographical question. As his doctoral thesis, Ewald asked Sommerfeld about the passage of electromagnetic waves in crystals, *etc.*

WF: In *electron lattices*.

TK: In *electron lattices*. Where did this dissertation appear?

WF: It was published in Munich, so it must have been printed in Munich.

TK: It was before the war, I think, and only an abridged version was published in the *Annals of Physics*. Where is the entire dissertation located?

WF: It has to be in Munich, in the archive, because he had to hand in several copies.

TK: When did he submit this dissertation?

WF: I don't remember that any more. Well, it must have been between 1912 and 1914, I don't know any more, around that time. If you just write to the Munich University Archives, you will receive that information.

TK: A very beautiful work.

WF: It's strange, isn't it, that Laue suddenly came up with the idea. Of course, he also dealt with X-rays, theoretically, didn't he, because they had a lot of analogies with optics because of how they originated and the Bremsstrahlung and natural radiation *etc.* So of course he knew something about X-rays and the unsuccessful attempts to observe X-ray diffraction experimentally, as was done by Haga and Wind,²⁹ who had done experiments with such narrow slits, that they could only ever propose an upper limit [for the X-ray wavelength]. If X-rays have a wave-like character, then the wavelength must be at most 10^{-9} .

JH [in English]: Was there any feeling at all at Munich in favor of the elder Bragg's³⁰ particle ideas for X-rays?

TK [Translating]: What did the physicists in Munich think of the Bragg corpuscular hypothesis?

WF: You didn't believe it, first of all, because some things were so terribly difficult to understand with this theory. Some properties of X-rays, for example, the energy of the electron that occurs when a – [Cigarettes offered and refused]. No, this theory was not correct. I have said this in my speeches about the discovery, and I have said so many times, not only in Munich but also before.

TK: Have your lectures on the history of the discovery appeared anywhere?

WF: Yes, they have appeared. That's when I made the point that it's a little bit humorous to hear that all the bosses didn't believe in crystal diffraction, and the student did it at night, you know? [Chuckle]. But it's actually the case that these things would not have been discovered at that time because the experiments were forbidden to be attempted by the bosses. Who was going to do it?

TK: Sommerfeld was also very negative?

WF: He was negative. Everyone was negative, and even Röntgen didn't believe it.

JH: Because of thermal vibrations.

WF: Yes, yes. You thought about the thermal vibrations, the atomic motions, they always move, there's no regularity.

JH: Did Epstein³¹ play any part in those discussions?

WF: Epstein was a guest at the university at the time.

TK: He didn't take part in the discussions?

WF: Yes, yes, yes. Afterwards he went to America, Epstein did. In my opinion, he was a very clever person, Epstein. I don't know, wasn't he in Los Angeles?

JH: Pasadena.

TK: Do you have any memories of people who attended the Sommerfeld seminar between 1910 and 1912? So it was you and Ewald, yes? Laue was there too?

WF: Laue was there too, then Lenz, Epstein – wait, who else? That was a long time ago.

TK: Röntgen was there regularly?

WF: Yes, he seldom came. Röntgen did not want to hear much about the – let's say – exclusively mathematical physics, for the simple reason that he knew the theories, the foundations of the physical phenomena, the laws, quite well, but he didn't have the mathematical tools, you know. So he didn't understand it if you were using vectors, or possibly tensors – these things we thought were really great – or matrices, right, he didn't understand that at all [Chuckle].

TK: But he was familiar with Maxwell's theory.

WF: It was known to him, yes, yes, of course.

TK: Boltzmann³² was in Munich, wasn't he? When was that? 1902?

WF: Yes, in 1902, I never knew him at all.

TK: Were a few Boltzmann traditions left behind?

WF: Only the armchair!

[Laughter]

TK: The style of the lectures *etc.* was not maintained at all?

WF: No, I think that happened in Vienna later.

TK: And his assistants at that time, they were not kept?

WF: No, no. The chair was empty for a long time. Sommerfeld was called only because of Röntgen. Röntgen was of the opinion that a chair for modern theoretical physics was required. We absolutely needed it because the other physicists who were there, such as Leo Graetz – I don't know if you are familiar with his book about physics and electricity, which was very nicely written, but of course old-fashioned. Röntgen had Sommerfeld fetched because he particularly valued Sommerfeld's theoretical work since it dealt with current problems in physics at the time, including quantum theory and related fields.

JH [in English]: Do you know what Röntgen's attitude towards quantum theory was?

TK [Translating]: What was Röntgen's opinion regarding quantum theory?

WF: Oh, he supported it. I'm sure he supported it. Röntgen supported all theories that, let's say, had some prospect of realization, so that one could, so to speak, use the concept to explain physical behaviors. That impressed him. He said: "All attempts to make a theory that can explain a phenomenon, I appreciate that, even if I don't understand the mathematical context completely."

TK: Were Röntgen and Sommerfeld friends?

WF: Yes, yes, they were friends. Röntgen was much older.

TK: When did he die?

WF: He died when he was 76 years old, when might that have been? I gave a memorial for him.

TK: It was during the war, no?

WF: No, not during the war. Wait, when did Röntgen die?³³ I really can't say. I gave a commemorative speech for him in Munich. I do not know.

TK: One more question: Did Sommerfeld read about thermodynamics?

WF: Yes, yes, yes. He was familiar with the whole field of theoretical physics.

TK: Did he also read about Maxwell's theory?

WF: Yes, yes, and thermodynamics, and optics etc. Above all, he taught his students using (analytical) mechanics so that they learned how to treat physical problems because he always had the point of view: "What I want to show you in my lecture is not how to differentiate or how to integrate or solve a differential equation, but how to take the proper approach." He said: "What use is it if you can differentiate and integrate, but if you don't know how to treat a falling stone? How do I deal with the case laws theoretically if I don't know how to treat them? Which approach do I take?" You know that's how it was in his seminars: The approach was the important part. That's what he demanded of his students, who had already had the mathematical lectures so that they could differentiate and integrate. But they mainly learned to approach a physical problem, and that's why he started with mechanics.

TK: ...Please, were Sommerfeld's lectures published?

WF: No, no, never. He wrote a few nice books.

TK: But later. Don't you have any notes or records, with his lectures?

WF: No. When Sommerfeld arrived, I was almost finished.

JH: What were the relations between Sommerfeld and Debye?

WF: The relationship between Sommerfeld and Debye was very good, actually. He liked Debye very much. He encouraged him a lot. He brought him to Holland and then to Zurich.

TK: Aachen too.

WF: Aachen first. Yes, I was pleased that Peter Debye was there last year at the 50th-anniversary celebration of X-ray diffraction. Yes, we greeted each other happily [Chuckle]. We had a very nice life together in Munich. As is customary, you go to a café after lunch, which is similar to Vienna. And we all met in the café, and there were, especially in the summer, tables that were made of stone – marble – and once the physicists left after drinking their coffee, the whole table was painted with formulas and drawings and figures etc. That was very nice. And then in the evening, after the colloquium, there was something else, we played skittles. We ate together, and we played skittles with Sommerfeld, you know, all physicists. That was a nice time. And also with the older students, who were working on their doctoral theses.

It was very difficult to do a doctorate with Röntgen. He gave very complicated assignments. Now, I'll tell you the task Paul Knipping was given for a doctoral thesis, the elastic response of diamond at high pressures and low temperatures. A diamond crystal was loaded, and the strain was measured with an interference device, interference bands, you know? And then the pressure was released, and the bands moved back but not all the way back. So that was the elastic response. The whole apparatus was in a

steel vat, and a pressure of 300 atmospheres was pumped in, and the whole thing was immersed in liquid air. Now do the experimental setup as a student [Laughter]. He spent four years on his doctoral thesis.

I also did work using X-rays. Yes, you had to make the X-ray tube yourself. So you went to the glassblower and got it done, and you had to make the pump and do everything yourself.

TK: What were the relationships like between Sommerfeld and his students? You just said that Ewald was having trouble with his doctoral thesis, and that he was very happy to discuss his issues with Laue. What was the relationship between Sommerfeld and his students? When Sommerfeld assigned a task to one of his students –

WF: Then the student didn't want to appear stupid, and as a result, he asked others for help [Laughter]. That was the reason, okay, that he didn't go to Sommerfeld. Otherwise, Sommerfeld would have said: "You don't know that?!" So the student went to Laue.

JH: Later, Sommerfeld had a reputation for talking at great length with his students.

WF: He did, sure, sure. But when he gave you a job to do, he'd say, "You can do it." But if you couldn't, then you didn't go to Sommerfeld but to someone else, with a little diplomacy [Laughter].

Röntgen was also a very strict gentleman. Oh! He gave me 30 glass plates one evening and said: "Mr. Friedrich, would you measure the thickness of these 30 glass plates tonight?" With an interferometer, you could measure it to the nearest micron. I measured 25 and thought I would measure the last five the next morning. So I arrived at my laboratory at 8 am, and His Excellency Professor Röntgen is already sitting there [Chuckle]. He is already sitting there, and he says: "Well, Mr. Friedrich, have you measured my plates?" [GH returns, Friedrich repeats the anecdote up to here.] I said: "I measured twenty-five last night, and now I want to measure the last five." "Well, how late did you stay up measuring?" I replied, "Well, until midnight." And then he said: "Well, and what did you do then?" [Laughter]. That's how it was!

Or, during the Carnival period – Munich celebrates the Carnival – you know what that is, Carnival?³⁴ – and so on Ash Wednesday I didn't arrive at the Institute at eight in the morning, and as a result, he promptly sent his mechanic to find out where I was. And there I am – I was still in bed – so I quickly got dressed on Wednesday morning at half-past eight and went to work. And he said: "I thought the Carnival was over! Why didn't you come to work? We can't have these lazy dogs!" [Laughter]. He said to me, "Well, next time–"

[End of interview]

¹This term is a direct translation of the German word *Elektronengitter* used by Friedrich in his interview. Readers will be aware that the use of the word *lattice* in this way is incorrect according to the crystallographic definition since the middle of the 19th century (see the [discussion](#)). It would be preferable to translate this perhaps as a *periodic array of electrons*. However, we retain it in this article rather than attempt to rewrite Friedrich's historical usage (comment from *IUCr Newsletter* Editor).

²Identified as Henri Bateau on the manuscript and Jacques Thibaud in his entry in the German *Wikipedia*.

³Wilhelm Röntgen (1845–1923), Professor of physics at the University of Munich from 1900 to 1920, discovered X-rays in 1895 and received the first Nobel Prize in Physics in 1901.

⁴Arnold Sommerfeld (1868–1951), Professor of physics and director of the Theoretical Physics Institute at Munich, was a mentor to many Nobel laureates.

5Paul Peter Ewald (1888–1985), doctoral student with Sommerfeld, the developer of the dynamical theory of X-ray diffraction (including the 'Ewald sphere'), and founder of the International Union of Crystallography in 1944.

6Ewald was hired at the Polytechnic Institute of Brooklyn as head of the Physics Department in 1949 and retired in 1959.

7Max von Laue (1879–1960), the recipient of the 1914 Nobel Prize in Physics for the discovery of X-ray diffraction, was a Privatdozent with Sommerfeld.

8Gustav Mie (1868–1957), Professor of theoretical physics at the University of Greifswald from 1902 to 1917, who developed equations to describe scattering of electromagnetic waves by colloidal particles ('Mie scattering').

9Identified as [H.] Starke in the original manuscript and presumably refers to Oskar Hermann Starke, extraordinary Professor of physics at Greifswald, who discovered secondary electron emission.

10Added parenthetically in the original manuscript but identities are uncertain.

11Wilhelm Wien (1864–1928), who studied black-body radiation (Wien's displacement law) and won the 1911 Nobel Prize in Physics.

12Following his X-ray doctoral studies with Sommerfeld, Knipping worked in the Siemens Laboratory in Berlin on Coolidge-type X-ray tubes. He was employed with the Kaiser-Wilhelm-Institut für Physikalische und Elektrochemie in Berlin-Dahlem. Eventually he became a Professor in X-ray physics at the Technical University in Darmstadt until his death in 1935.

13William Lawrence Bragg (1890–1971), co-winner of the 1915 Nobel Prize in Physics with his father W. H. Bragg for their transformative studies of X-ray crystallography.

14Presumably, this refers to the Heraeus Group, an industrial chemistry company founded in 1851 that refined techniques for melting platinum and manufacturing quartz glass.

15Curiously, they missed the fact that diffraction from diamond went against Laue's original supposition of the need for secondary X-rays (*IUCr Newsletter* Editor).

16Otto Lehmann (1855–1922), head of the Institute of Physics in Karlsruhe, performed early studies on liquid crystals.

17Peter Debye (1884–1966), winner of the 1936 Nobel Prize in Chemistry, made major contributions to both theoretical and experimental solid-state physics, including the Debye–Scherrer powder camera mentioned here.

18Perhaps this statement refers to the letters from Stark.

19Laue shared the financial portion of the Prize with Friedrich and Knipping.

20Spelled without the 'e', this likely refers to Johannes Stark, a Professor of physics at Aachen University from 1909 to 1917 whose work on the shifting and splitting of spectral lines of atoms and molecules due to the presence of an external electric field earned him the Nobel Prize in Physics in 1919. His staunch Nazism resulted in a four-year suspended sentence for crimes against humanity following World War II.

21Allgemeine Elektrizitäts-Gesellschaft, the General Electric of Germany founded in 1883.

22Bernhard Krönig (1863–1917) was a Professor of Gynecology at the Freiburg University Clinic, who with Friedrich pioneered the exploration of the effects of ionizing radiation on human tissue.

23Friedrich Dessauer (1881–1963) studied physics at the Technische Universität Darmstadt and the University of Munich, with a focus on the medical applications of X-rays. His face was severely disfigured from radiation damage, and he was imprisoned in the 1930s for his opposition to Hitler.

24Boris Rajewsky (1893–1974) was a Rector at the Goethe University in Frankfurt and was highly honored for his studies of the effects of radiation on organisms.

25Leo Graetz (1856–1941) was a Professor of physics at the University of Munich who studied the propagation of electromagnetic energy.

26Wilhelm Lenz (1888–1957) rose to Professorships in physics at the Universities of Munich (1920), Rostock (1921), and finally Hamburg (1921–1956) and is recognized today as the originator of the Ising model.

27The notion that crystals embodied atoms or molecules organized by a space lattice was widely shared among mineralogists of the time. von Groth's own 1906 text approvingly cites the application of early space group theory to crystals by Leonard Sohncke, Professor of physics at the Technical University of Munich from 1886 to 1897.

28von Groth (1843–1927) was one of the most pre-eminent mineralogists of the day, having founded the journal *Zeitschrift für Krystallographie und Mineralogie* and developed a five-volume systematic mineral classification.

29Hermanus Haga (1852–1936) was a Professor of physics at the University of Groningen from 1886 to 1921, and he collaborated with Cornelis Wind (1867–1911) to determine the wavelengths of X-rays by passing radiation through a V-shaped slit that was 27 μm at the top and close to 0 μm at the base. The broadening of the detected intensities from the narrow portion of the slit was interpreted as evidence for X-ray diffraction.

30William Henry Bragg (1862–1942) developed some of the first effective X-ray spectrometers and firmly believed in a particle-like nature of X-rays until his son's experiments convinced him otherwise.

31Paul Sophus Epstein (1883–1966) was a Russian-born mathematician and physicist who worked with Sommerfeld in Munich before ultimately becoming a Professor at Caltech. A member of the US National Academy of Sciences, he explained the Stark effect using quantum theory.

32Ludwig Boltzmann (1844–1906), the father of statistical mechanics, was Chair of Theoretical Physics at the University of Munich from 1890 to 1894, at which point he moved to the University of Vienna, so the recollections are amiss here.

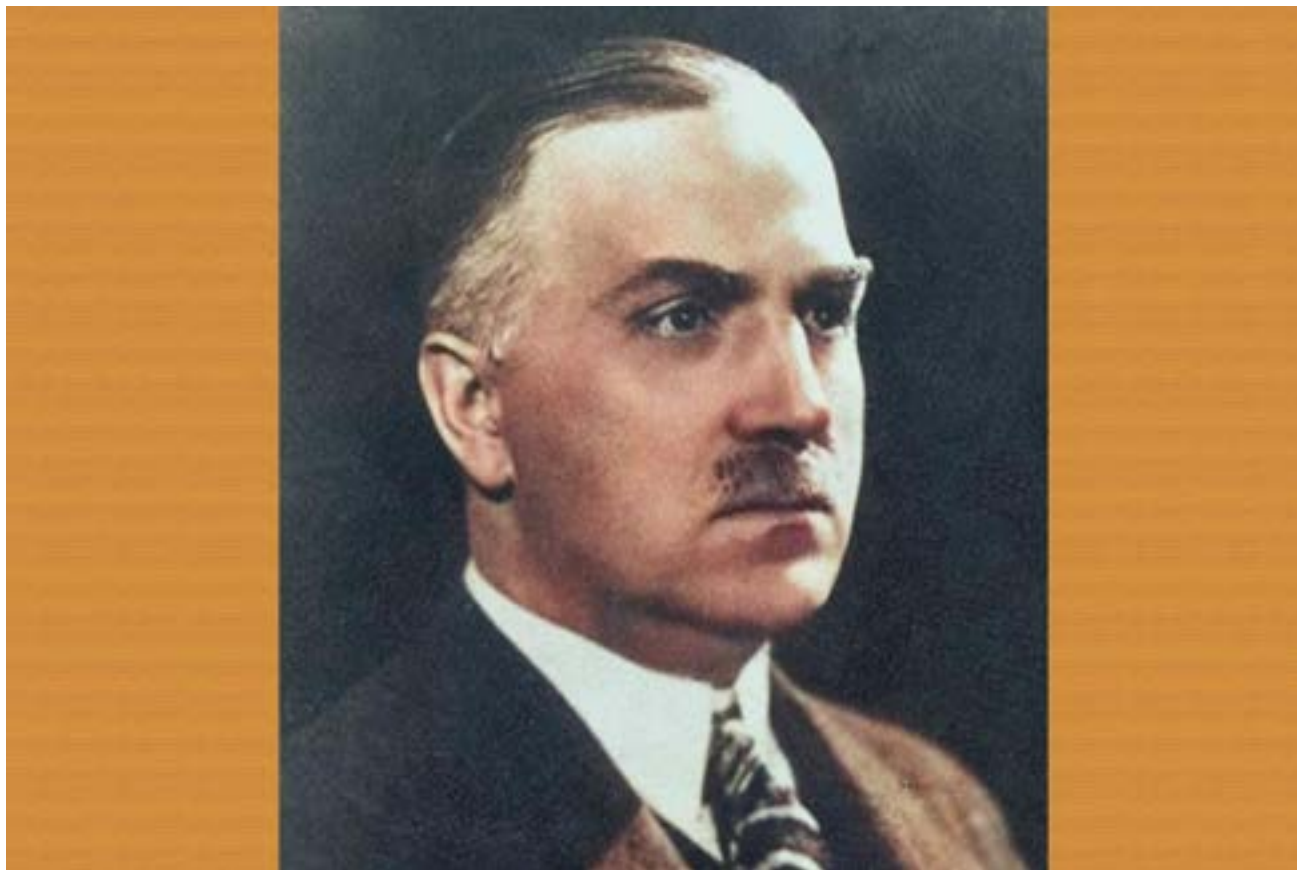
33Röntgen died in 1923, one-and-a-half months shy of his 78th birthday.

34The Christian Carnival celebration in Germany begins with the feast of the Epiphany (Three Kings Day) and ends on Shrove Tuesday, the day before Ash Wednesday.

HISTORY OF CRYSTALLOGRAPHY

Who was Jan Czochralski? Out of the shadows

Mike Glazer



For those working in the field of crystal growth, the name Czochralski is well known as a particular technique, the Czochralski method, whereby a large pure crystal can be pulled from a molten substance. This is the standard method, for instance, for growing huge crystals of silicon and germanium, as well as many other crystalline materials of interest. The importance of the Czochralski method can, therefore, not be overstated as so much of the modern world depends on being able to grow Si/Ge crystals on an industrial scale.

But who was Czochralski and what did he actually do? His story is interesting and mysterious, the stuff of movies. It is a story of discovery and tragedy set against the events in Poland and Germany in the 1930s and 40s. The following account of his life has been adapted from a lecture I gave a few years ago in Kraków, Poland. The book *Jan Czochralski Restored* by Paweł Tomaszewski (2013) provides much more detail than is possible in this short article. I shall try to highlight the significant events of his life here, a story that is now well known in his country of origin, Poland, but somewhat overlooked elsewhere.

Early Life and Career

Jan Czochralski was born in 1885 (Fig. 1) in a small town called Kcynia (Exin in German) near the Polish city of Poznań. At the time, this part of present-day Poland was in the Prussian partition (from 1772 to 1795 Poland had been partitioned between Prussia, Austria and Russia, only regaining its independence

in 1918). So officially, Czochralski was a citizen of Germany. The question of his 'Polishness' became an important matter for him many years later, as we shall see.

A.

Nr. 84Exin, am 21. October 1885

Vor dem unterzeichneten Standesbeamten erschien heute,
der Persönlichkeit nach _____

_____ ^{be} kannt,
die Verheiratete Frau (F. Francine)
Crochmalsti

wohnhaft zu Etia

Katholischer Religion, und zeigte an, dass von der
Maria Crochmalsti geborenen Lu-
thomische, seiner Ehefrau

Katholischer Religion,
wohnhaft bei ihm

zu Etia in seiner Wohnung

am dreizehntzigsten October des Jahres

tausend acht hundert acht zig und fünf Uhr am Freitag

um vier Uhr ein Kind weiblichen

Geschlechts geboren worden sei, welches den Vornamen

Joseph (Jon)

erhalten habe

Vorgelesen genehmigt und unterzeichnet

gog. F. Crochmalsti

Der Standesbeamte.

gog. Krapfner

Figure 1. Jan Czochralski's birth certificate. Technically, a German citizen under the Prussian partition. Although note that his father's name was written both in German and Polish ('Franciszek').

It seems that little is known about Jan's early years or his time at school. Curiously, no evidence has been found of him gaining the so-called '*matura*', the expected qualification needed for university studies in Poland. It is known that Jan travelled to Berlin (Fig. 2), where he worked from 1907 to 1917 at the Kabelwerk Oberspree cable factory (AEG), as an assistant to the German engineer Wichard von Moellendorff. During this time, he worked on introducing aluminium into electrotechnology. But it was here that he made a momentous discovery. The story behind this is legendary and there are several versions of it. But it goes something like this.



Figure 2. Czochralski in Berlin in 1907.

Discoveries

It was 1916, during World War I. One more working day was coming to a close and the laboratory had emptied. Jan was sitting at a table to complete the researcher's routine: writing down the results of the day's work. He was tired and preoccupied; for weeks, he had been searching for a way to measure the crystallizing speed of metallic alloys. The war restrictions on material supply were being felt more and more painfully. So the industry was urgently in need of some substitute materials, such as metal alloys, which could replace the traditional ones used until then.

Probably from being tired, Jan absent-mindedly dipped his pen into a pot of molten tin that was cooling off, thinking it was the ink well. He noticed a thin thread of metal hanging off the pen. Quite preoccupied, he changed the nib, putting a new one in, and carefully immersed the pen into the melting pot. Then he slowly pulled it out, and once again, he saw a hanging thread. He continued with another nib. The same thing happened. So he took one more nib. It was just the same. Having broken off the metal thread, he dipped the pen again in the melted tin. This time he pulled it out briskly: the thread was not there. Interesting....

Jan failed to notice that the sun had long stopped peeping into the lab through the windows. He was so absorbed 'playing with' the tin thread, pulling it out of the melting pot. Could it be so that the length of the thread depended on the speed with which he pulled the pen out? 'So I've found a solution' he thought. Could that be some property of the metal?

A series of prompt, yet systematic, experiments demonstrated that the quicker he pulled the pen out, the shorter the thread was. Jan swiftly wrote this observation down so as not to forget this interesting relationship. He spent the following days working out a device that would help to more objectively test whether his accidental observation implied information about the material's properties (Fig. 3). He knew from Gustave Tammann's¹ previous studies that crystallization occurred in a small hole of a thin glass tube. The incision on the nib of his pen served like such an open capillary. The hand had to be substituted by a mechanism to lift the tube at a chosen fixed speed. At first, he used a clockwork motor (Fig. 4).



Figure 3. Left: Czocharski's 1916 paper on a method for measuring the rate of crystallization. Right: Czocharski in the AEG chemical workshop of the metal laboratory in 1911 [photo from the work of von Moellendorf (1911)].

The news of Czocharski's discovery² travelled fast among his colleagues. It must have been an important one as they could not have read about it by then, as the first scientific information was printed only in 1918. Soon one more benefit of the crystallization speed measurement method was observed: the acquired metal thread was a single metal crystal. This provided the opportunity so many scientists had been dreaming of as they were aware that testing many metal physical properties was possible only on single crystals. Several years before, W. H. Bragg and his son W. L. Bragg had demonstrated that a monocrystalline solid is built of atoms arranged in an almost perfect way. Yet, prior to Czocharski's discovery, a method of obtaining metal crystals simply and cheaply was unavailable. Thus, metallurgists were given an excellent tool for producing such materials, namely the Czocharski method. Interestingly, he did not patent the technology nor benefit financially from it. He may not have realized at the time the importance of this method, as it was other scientists later on who noticed that it could be used to grow large crystals.

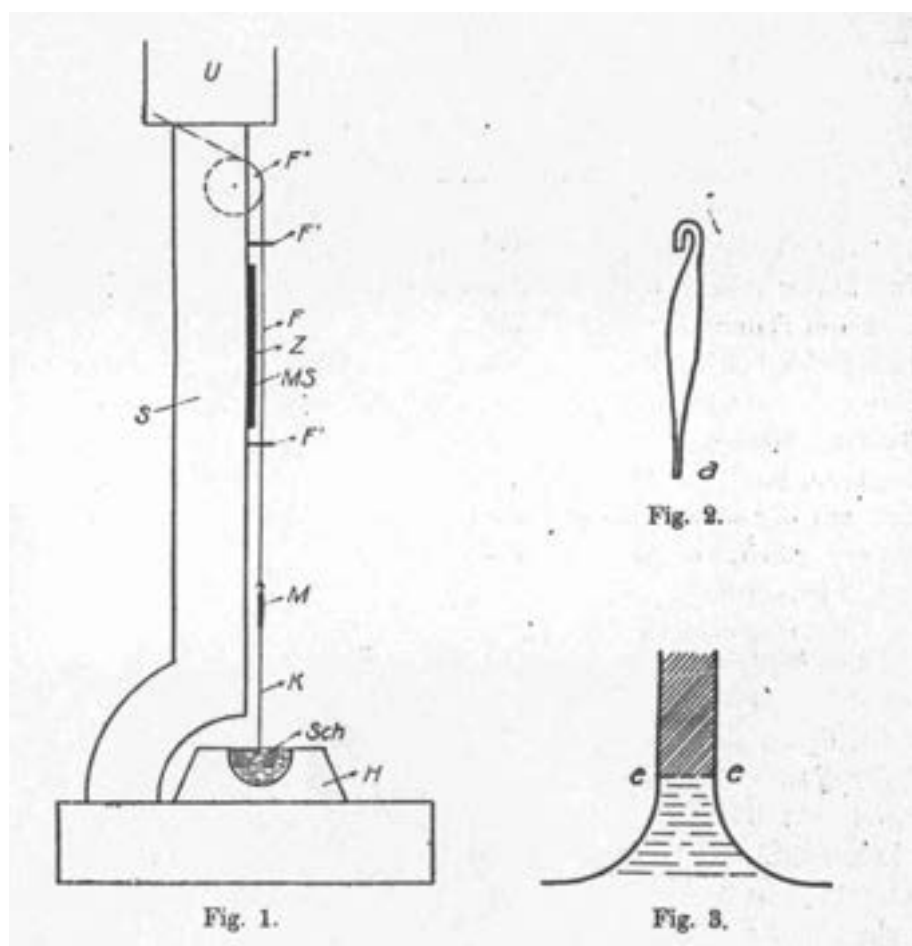
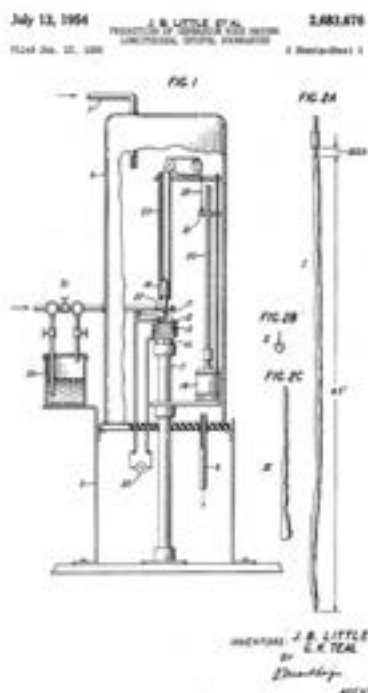


Figure 4. Czochralski's drawings of his original crystal-pulling apparatus.

In particular, it was Gordon Teal working at Bell Labs in the 1950s who modified Czochralski's method to grow large crystals of silicon and germanium for the first time. The 1955 patent (Fig. 5) by Little and Teal does not mention Czochralski's name but starts with the statement: "*This invention is related to an improved method and apparatus for producing single crystals, particularly of germanium.*" Despite this, it is Czochralski's name that is universally used to refer to this method of crystal growth. In addition to the growth of silicon and germanium, the Czochralski method is the leading technique for growing many other crystalline materials of interest, such as high-quality bulk oxide crystals. Whereas many semiconductors are now grown by epitaxy, there is still a need for high-quality oxide crystalline substrates.³



**300 mm diameter, 2m long
265 kg**

Figure 5. Left: 1955 patent of Little and Teal, Bell Labs, for the growth of semiconductors germanium and silicon. Right: An example of a large boule of germanium grown using the Czochralski technique.

In 1917, Czochralski moved with his family (Fig. 6) to Metallbank u. Metallurgische Gesellschaft A.G. in Frankfurt am Main to found a new large laboratory, one of the best-equipped laboratories then in Germany. Here he invented a new metallic alloy called B-metal (German: Bahnmetall) used to make high-quality elements of bearings for the railway industry. It was cheap, very durable, and, most importantly, did not contain tin, which was expensive and hard to get at the time. By 1928 he was now famous and wealthy thanks to his income from this patent.



Figure 6. Jan Czochralski and family in 1923.

Another invention during this time is intriguing. In 1925, he built a device that he called a radio microscope (Fig. 7). It had already been discovered in the 1870s that the contact of a metal with a semiconductor displays rectifying properties. This allowed one to build semiconductor elements, so-called 'crystals'. Czochralski's idea was based on the old crystal radio sets where a needle was moved across a crystal to maximize the received radio signal. In his device, he scanned a copper needle across a polished aluminium wafer containing silicon inclusions. The radio microscope included an antenna to pick up a radio broadcast (later when working in Poland, he tuned it to the Polish radio station Raszyn). Whenever the needle met a silicon point, because of rectification, there was a change in the intensity of the radio signal. These points were then plotted to produce a map of the inclusions. This is the description in Czochralski's own words:

"Thus, if on the one hand, you connect the antenna with the alloy, while on the other silicon crystals are touched with a sharp needle connected with the phones, thus making the current flow through the phone's coil to the ground, such a system should affect the course of electromagnetic waves like every detector. What can be seen in the scheme is: any antenna whose current flows to the metal detector table serving as the sample base and to the microscope placed on the table. The researcher's needle, also metal, is joined with the phones' clips by means of an appropriate conductor. A rectified antenna current flows further on through the coils to the ground. When the needle touches a silicon crystal, once the electromagnetic waves reach the antenna, a sound is heard in the phones. (...) One can easily make the receiver in such a way that it is tuned merely to a particular wavelength (all we need thus is an induction coil of variable self-induction to be added into the oscillating circuit as marked in the sketch with the dotted line and the circuit tunes to a given wavelength) (...)".

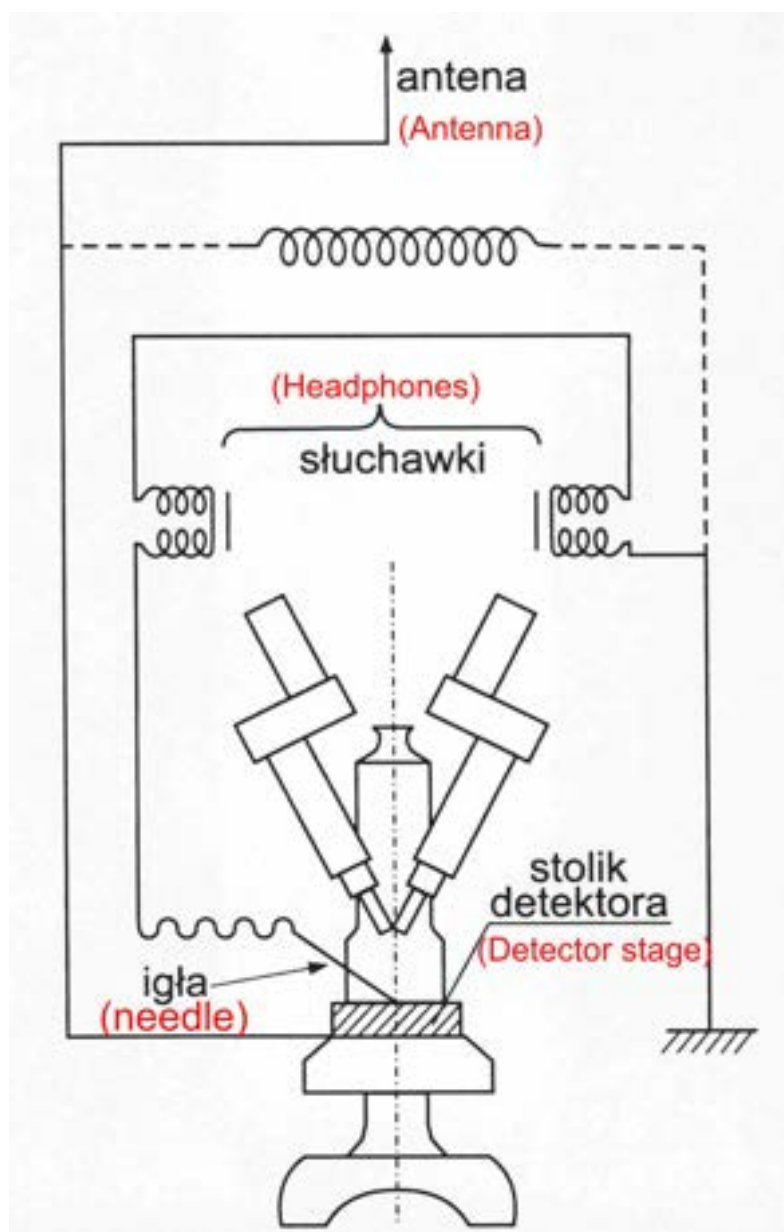


Figure 7. The radio microscope 1925.

Now, where have we seen a similar idea that many years later gave rise to a Nobel Prize?

Another area of research was recrystallization methods. For instance, he discovered that when annealed metal strips are stretched slightly at an appropriate temperature, recrystallization is induced, with crystals many centimetres thick and relatively free from crystallographic defects. In 1923 he was the first to publish in Poland an X-ray diffraction study of a single crystal and was soon demonstrating crystal structure models to visitors.

Poland

After all his successes in Germany, the story then takes a twist, which would later turn out to be cataclysmic. In 1928 he went with his family to Warsaw at the personal invitation of the President of Poland, Professor Ignacy Mościcki, himself an outstanding chemist. Czocharlski later said: *"I was tempted to return to Poland, (...) as my children were growing up and I wanted to send them to a Polish school so as not to let them become Germanized!"* (Fig. 8).



Figure 8. Left: Czochralski with wife and daughter. Right: Czochralski's home 4 Nabelaka Street, Warsaw, now the residence of the Ambassador to Slovakia.

In 1929, Czochralski was appointed Professor at the Faculty of Chemistry of the Warsaw University of Technology (Fig. 9) and was one of the first to be conferred with the University's honorary degrees. This was despite not having the usual formal qualification of the Polish *matura*, something that caused some in the University to look askance. At the University, he set up his own Institute of Metallurgy and Metal Science (Fig. 10) with significant state funding and a large number of staff. By all accounts, his institute was self-contained and seemed to act independently from the rest of the university. Unsurprisingly, this must have led to considerable jealousy among certain members of the University Faculties.



Figure 9. The Chemistry Faculty of the Warsaw Institute of Technology 1939. Czochralski sits in the front row on the far left (anyone who has attended the EMRS meetings will recognize the background in the main hall).

In the period 1934–1938, Czochralski became embroiled in a series of court battles, such as when he was accused of defamation by the metallurgist Professor Witold Broniewski and accused about the usefulness of B-metal (Broniewski argued that its use would cause the stoppage of railway transportation). Generally, these cases had their origin over the question of Czochralski's lack of official qualifications and questions about his citizenship (was he German or Polish?) and patriotism to Poland. Eventually, the courts found in Czochralski's favour. On 19 October 1936, Broniewski was sentenced by the [District Court in Warsaw](#) to a two-month suspended arrest and a fine of 500 złotych in a defamation trial brought by Czochralski. In December 1938, the Supreme Court upheld the above judgments.



Figure 10. The current view of the Chemical Technology Institute. Czochralski's office is circled.

At the institute over a period of years from 1930 onwards, much new equipment and facilities were added, some for research into materials for military armaments and some for civilian use. In May 1939, shortly before the German invasion of Poland in September, the physicist and later Nobel Laureate Professor Walther Gerlach (1889–1979) from Munich judged Czochralski's institute to be better equipped than many German institutions of its kind, despite having been shown merely its civilian part. A report to the Nazi Party Unit NSDAP, Berlin:

"In April, I received an invitation from the Director of the Institute of Metal Sciences of the Warsaw University of Technology, Professor Czochralski, additionally inviting me to stay in his house. I have known Professor Czochralski for 20 years; we were on especially friendly terms at the time when he headed the research laboratory of Metallgesellschaft in Frankfurt, and I was working at the University there. We cooperated a lot and have remained friends since. Despite being away, Professor Czochralski came briefly to Warsaw (...).

I had the opportunity to visit the Metal Science Institute of the Warsaw University of Technology only partially. Some of its sections are closed to visitors, as they are controlled by the army, since, like in many German institutes there too, Polish professors are working on the issues of state importance. What I saw in the Institute ranks among the most beautiful things I had ever seen, and which in Germany can

only be found in industry research institutes. The Institute is housed in a large several-storeyed building raised for the purpose some years ago. It contains all the possible devices for experiments and auxiliary means for pure metal science, metal chemistry, metal physics and metal technology (working). It seems to me that it is mainly a research institution, but it is also involved in teaching; for teaching purposes, it has first-class aids and devices. I cannot tell the actual size of the Institute, yet I assess that it is four times as big as the new KWC Institute of Professor Debye in Dahlem. It seems likely that the (Warsaw) Institute enjoys substantial financing. Its studies are published in its own publications having some hundred pages annually. All the studies are almost exclusively written in Polish, with extensive abstracts in German, English or French.

In my judgment, the Institute focuses on strictly academic issues: alloys, steel hardening, light metal improvement: also some scientific-technological issues: investigating metals, corrosion, etc. There also must be some target-specific research carried out. Apart from specialized research apparatuses, I have also been shown apparatuses for series tests on a large scale.

(...) In brief, I can say that despite the political tensions, the trip went on undisturbed (...) Politics was entirely excluded from our talks; all we did was express the desire that this visit could be followed by further scholarly contacts."

World War II

A result of Gerlach's report was that it helped the occupying forces in the destruction of the laboratories, as they knew what equipment and facilities existed. Under German occupation, all high schools and universities were closed down, yet Czochralski was able to set up a new technical laboratory using the Institute's equipment and people.

From time to time, senior Nazi officials were seen to visit him, e.g. on 4 November 1939 the Institute was visited by SS Hauptsturmführer Professor Heinrich Harmjanz of Einsatzkommando⁴ IV der Sicherheitspolizei Warschau, who reported:

"It is a huge Institute equipped with the most modern apparatus and was financed mainly by the research resources of commissions placed by Polish industry. It employed 85 paid employees and assistants. The head, with fluent German, worked for some dozen years in German industry and personally became acquainted with many German plants. He informed me that, until the outbreak of the war, he had maintained wide contacts with German industrial plants. He told me that he had already expressed to Dr Fischer, head of the Warsaw District civil administration, his readiness to cooperate with the Hermann Göring State Works. Apparently, Dr Fischer considers the possibility of using the Institute for a four years' plan of Poland's economic recovery as worth analyzing."

The activities of Czochralski during this period were complicated. They have been fully documented by Tomaszewski and will not be described here.

During German occupation of Warsaw, ever more restrictions on daily life were imposed on the population. Despite this, Czochralski apparently continued to live a lavish life in his villa, where he held receptions and collected artworks. The Jewish population of Warsaw was moved into a confined area of the city, the so-called ghetto. Many died of starvation and disease or were sent to the death camps. Finally, on 19 April 1943, an uprising began by the remaining ghetto population. Although being poorly equipped and small in number, the Jewish resistance was able to hold out until the final defeat on 16 May, followed by the wholesale destruction of the ghetto area. The following year from 1 August until 2 October, the Warsaw Uprising took place, which resulted in massive destruction of the city.

It is known that, in early September 1944, Jan lived in Milanówek (just outside Warsaw). After the Warsaw Uprising, the Nazis ordered the transportation of the property of the blockaded and ruined city. Czochralski, as the head of the Materials Research Unit, was also involved, on the German authorities' instruction, in transporting precious apparatus of the Institute. As a rule, people deviated from the

marked route to save something from their own or a friend's flat. The latter, however, was not always possible (when the transport was accompanied by a German soldier), or was not necessarily safe if the Nazis were to find among the possessions something outside the pass list. Very often, the evacuation was a paid procedure: most likely, money was paid to the transporting team and bribes were paid to the guards controlling the vehicles leaving Warsaw.

Ignominy

On 7 April 1945, after the Germans had left, Czochralski's tragedy began. On that day, the Prosecutor of the Special Criminal Court for the Court of Appeal in Warsaw announced the arrest of "*a certain Jan alias Johann Czochralski, a citizen of the Reich, former honorary Professor at the Warsaw University of Technology, who after the Warsaw Uprising was supposedly dwelling in Piotrków.*" This was in compliance with the so-called August Decree, namely the Decree of the Polish Committee of National Liberation of 31 August 1944 "*on the Sentence for Nazi Criminals Guilty of Assassination and Torturing Civilians as well as War Prisoners and for Traitors of the Polish Nation.*" Several people spoke up for him, where one of the issues considered was whether he was a Pole or German. This was a complicated matter⁵, as he constantly maintained his Polish identity despite having been born under Prussian rule. Fortunately, the investigation proved that Czochralski's activity during the occupation did not show symptoms of collaboration with the Nazis and therefore could not be classified as a "*betrayal of the Polish nation.*" Such was the Prosecutor's conclusion, and so the investigation was dismissed for lack of evidence. He was released from prison on 14 August 1945.

At the Warsaw University of Technology, members of the Senate declared "*as of the end of 1939 Dr Jan Czochralski ceased being considered by the Professors' body of the Warsaw University of Technology as a Professor of the Warsaw University of Technology and decides to respond that J. Czochralski's intention to work for the University of Technology is not valid*". Thus Czochralski's name was erased from the list of Professors. Czochralski took the Senate's decision as his personal failure and humiliation. Despite having been proposed to emigrate to Austria and take a chair in Vienna, he and his wife returned to Kcynia. There he founded a small company BION producing health products, cosmetics and household chemicals. The rest of his life was doomed to infamy and oblivion. He died from heart failure on 22 April 1953.

The actual circumstances that led to the death of Czochralski at the age of 67 remain unclear. According to one version, it came as the result of the intrusion of officers of the infamous 'U.B.', Secret Police, searching, in compliance with some denunciation, hidden dollars from the sale of his house in Warsaw. However, they were unable to find anything. Terrified at the vision of wreckage of his house, Czochralski revealed to them an ingenious hiding place in a window ledge. His 20-dollar golden coins were thus lost, and the price for that was highly paid: a heart attack. According to a second version, the heart attack happened later: it was supposed to have occurred after chasing some boys vandalizing his garden. His grave remained nameless for 45 years. Even here, mystery is attached to Czochralski's life.

The secret

So, this is how the Czochralski story remained during the long years of the Communist government in Poland. During this time, mention of his name was actively discouraged. It was clearly of great sensitivity to the then Polish authorities. However, some academics, including Tomaszewski from the Polish Academy of Sciences in Wrocław (before the war Breslau), began to investigate Czochralski's history. I recall that at the European Crystallography Meeting in 1986 held in Wrocław, Tomaszewski wanted to hold an exhibition on Czochralski's works and to invite a Czochralski expert to give a plenary lecture at the opening of the conference. However, mention of Czochralski was still a sensitive matter, and after receipt of various telephone threats, the lecture was given quietly in a rather nervous and tense atmosphere late one afternoon. But in 1989, the Communist government fell and a fully democratic

government took power. Suddenly, under the new President, Lech Wałęsa, it became possible to talk openly about Czochralski, and, importantly, to discover more of his life from secret archives.

Subsequently, the following are some of the discoveries:

- In 1941 the Germans demanded Czochralski's help to provide materials and equipment for their war effort. In fact, the demands for weapons were never actually fulfilled. He claimed that his Unit was overloaded with work.
- There is evidence of underground activity. Czochralski was given authority to provide employment certificates, and he gave many such permits to fictitious employees who were members of the Home Army.
- Together with his daughter, he was able to use his influence with the German authorities to intervene to release some people from concentration and POW camps.
- There is evidence of the manufacturing of arms for the Home Army (e.g. grenade shells).
- There is evidence that he sheltered two Jewish women in his home until the Warsaw Uprising.
- The German authorities managed to import a vital piece of American equipment with the help of the Swedes. When the apparatus finally arrived, Czochralski used a hammer to smash its essential component without which it could not operate.
- There is some evidence that Czochralski was instrumental in financially helping a previously owned Jewish business in the ghetto.

Czochralski recalled: *"During the occupation, I lived in Warsaw in my own villa of 16 rooms at 4 Nabelaka Street. I lived there only with my family made up of 6 individuals; apart from us there lived 2 Jewish women who stayed with us until the Uprising. In total, there were 10 individuals living there. On several occasions the Nazis wanted to occupy the villa, which they eventually failed to do. I suppose that my name being well known in science accounts for it."*

Interestingly, a photograph (Fig. 11) has been found of Czochralski attending the burial of an insurgent in the grounds of the Warsaw University of Technology. Incidentally, a few years ago, during a visit to the University for a meeting of the European Materials Research Society (EMRS), I was able to take a photograph (Fig. 12), which I think is at the same spot.



Figure 11. An insurgent's funeral on the University of Technology campus between 12 and 16 August 1944. From the left: Chaplain of the 3rd Armoured Battalion of the Home Army 'Golski', Camillian Mieczysław Mielecki, nom de guerre 'Mieczysław'; N.N.; and Professor Jan Czocharlski. Photo taken by Tadeusz Bancler, Battalion's photographer (from E. Bruliński's collection).

There remain other questions that have never been answered. Intriguingly, one has to ask why did President Mościcki invite Czocharlski to Warsaw in 1928 and why was he, despite lacking the *matura*, made a Professor and given his own institute with full funding? Could it be that he was working all along for the Polish secret service?



Figure 12. Present day Golski memorial in the Warsaw University of Technology to the defenders of the Polytechnic in the Warsaw Uprising.

Anyway, the result of all this is that, after much discussion, Czochralski's name was fully rehabilitated. On 7 September 2011, at the Congress of Physicists in Lublin, delegates of the Polish Physical Society adopted a resolution to appeal to the Polish Parliament to make 2013 the Year of Czochralski, as that year would be 60 years since he passed away. After some discussion, the Parliament declared 2013 as the Year of Jan Czochralski. The Senate of the University voted to restore his name to the list of Professors, and now each Fall meeting of the EMRS includes the presentation of a gold Czochralski medal (Fig. 13) to a distinguished materials scientist. Today, Czochralski is regarded as a national hero (Fig. 14) and he has finally emerged from the shadows. I understand that this year, Polish television will be screening a film about his life and achievements.



Figure 13. Czochoński gold medal of the European Materials Research Society.

In 2003, the then President of Poland, Aleksander Kwaśniewski, stated:

"During the tragic times of the Nazi occupation, he demonstrated great courage and righteousness. He was involved with the Polish underground, he supported the fighters of the Warsaw Ghetto, and participated in the efforts to save museum collections of national culture. It is for this attitude that, following WWII, he suffered unfair accusations, which, though ungrounded, made it impossible for him to work at University. He was an individual of exceptional merits. A noble patriot, a devoted son of his Homeland."



Figure 14. Two postage stamps celebrating Jan Czochralski. On the right marking the Year of Jan Czochralski.

With especial gratitude to Dr Paweł Tomaszewski, Institute of Low Temperature and Structure Research of the Polish Academy of Sciences in Wrocław, whose untiring perseverance to uncover the truth about Czochralski, sometimes under difficult circumstances, finally paid off!

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1 Gustav Heinrich Johann Apollon Tammann (1861–17 December 1938) was a prominent [Baltic German](#) chemist-physicist who made important contributions in the fields of glassy and [solid solutions](#), heterogeneous equilibria, crystallization and [metallurgy](#).

2 An excellent example of the wisdom of Pasteur's famous quote: "*Dans les champs de l'observation le hasard ne favorise que les esprits préparés*" ("*In the fields of **observation** chance favours only the prepared **mind***").

3 In 2019, Darrell Schlom, Cornell University (USA), and Reinhard Uecker, Leibniz Institute for Crystal Growth (IKZ, Germany), jointly received the Frank Prize of the International Organization of Crystal Growth for their pioneering contributions to the development of new perovskite substrates enabling strain engineering of functional oxides.

4 The Einsatzkommando were part of the so-called Einsatzgruppe (killing squads) and consisted of SS and Gestapo functionaries. There is evidence that Harmjanz (1904–1994) and his staff were active in the looting of museums, churches and mansions in the annexed territories.

5 A full account of this aspect can be found in Tomaszewski's book.

Please note that black and white images in this article have been artificially colourized by Photomyne.com.

AWARDS AND PRIZES

Olga Kennard awarded 12th Ewald Prize



The 12th [Ewald Prize](#) has been awarded to Olga Kennard (Cambridge, UK) for her invaluable pioneering contribution to the development of crystallographic databases, in particular the Cambridge Structural Database (CSD), which as she early foresaw, has led "... to the discovery of new knowledge which transcends the results of individual experiment". Her own surveys using the CSD were fundamental in the development of crystal engineering, and are outstanding examples of the use of crystallographic databases as an essential tool for analysis and prediction. As founder of the CSD, director of the Cambridge Crystallographic Data Centre (CCDC) over decades, and being involved in the founding of the Protein Data Bank (PDB), Olga Kennard has made a fundamental impact on the development of modern crystallography.

A small delegation, including the IUCr President, Sven Lidin, and IUCr staff, will present Dr Kennard with the Ewald Prize once COVID-19 restrictions are lifted, and a representative will deliver Dr Kennard's Ewald Prize Lecture during the Prague Congress Opening Ceremony on 14 August 2021.

Dr Kennard told the IUCr that she is "enormously grateful for this, totally unexpected, recognition - through the Ewald Prize - of both my own work and the contribution of the many scientists who collaborated with me over many years," and provided the following account of her life and work.

I was born in Budapest, Hungary, and lived there until August 1939, when we moved to England, just two weeks before the outbreak of the war. Although I spoke very little English, I was accepted at the Hove County Grammar School, and unexpectedly placed straight into the fifth form to matriculate the same year. I am not sure how I managed to pass all subjects, except English, and was able to continue to the sixth form at a grammar school in Evesham. I chose science primarily because it was the only constant between what I was taught in Hungary and in England. The arts appeared very different. Education and

learning were very important in my family, with no distinction between boys and girls and I was well supported when I decided to try and get into one of the two women's colleges in Cambridge. I was fortunate to be accepted at Newnham or, as my tutor told me later, managed to talk myself into college. There, in addition to three other subjects, I opted for mineralogy, a subject new to me. It was mainly classical mineralogy with very little mention of X-ray crystallography.

Two years later, having taken a wartime degree, Max Perutz took me on as his assistant and I actually became a co-author of an early paper on haemoglobin. Alas I was not permitted to try for a higher degree and only became a respectable scientist much later with a Cambridge ScD. It was the only time in my career that I met discrimination as a woman. The crystallographic community was extremely supportive and had many eminent and wonderful female crystallographers, who greatly helped me.

My path took me from laboratories in London back to Cambridge, where in the Department of Chemistry I started the Chemical Crystallography group in 1962 and the Cambridge Crystallographic Data Centre (CCDC) in 1965. As a working structural crystallographer I had a wonderful time solving increasingly complex structures as instrumentation and computing became more and more powerful, so that at the end of my time in the lab we were able to solve the structure of a fragment of DNA with a base-pair mismatch to 1 Å resolution!



Olga Kennard (left) with Paul Peter Ewald at the Ninth IUCr Congress in Kyoto, Japan, in 1972.

My involvement in the data field started in 1948, when J. D. Bernal became the first Chairman of the IUCr Commission on Crystallographic Data and asked me to be the Secretary. The CCDC was originally set up as the British contribution to an international effort aimed at preventing any one country acquiring a monopoly of scientific data. My involvement with the development of the CCDC and the use of structural data is fully described in a talk I gave at the [50th Anniversary of the CCDC](#) in 2015. Fortunately I didn't have to include the Protein Data Bank in the talk, although Max Perutz asked me, on behalf of the protein crystallographers, to set that up but much to my relief it was eventually taken over by others. The third databank I influenced was the Nucleic Acid Sequence Database, which I persuaded the European Molecular Biology Organization to embark on.

How do I see the future of the Cambridge Structural Database? Unstoppable probably, since even though we know a great deal about the formation and structure of crystals, the drive to solve more and more "small molecule" structures is still on and purely theoretical structural predictions are not likely to take over from good experimental data. At present I cannot anticipate the time when such data could become superfluous.

You ask about the Fellowship set up in my name by the Royal Society where special provisions are included for women. This was influenced by the terms of the Dorothy Hodgkin Fellowships and not by my own experience of bringing up two daughters as a full-time scientist.

On my retirement, as you noted, I became a Trustee of the British Museum. It was a wonderful experience to work at such a great institution and with an inspiring Director, Neil McGregor. We were also involved in building a new extension to the Museum, which was of great interest to me having been involved in architectural projects, such as the award-winning CCDC building, and being passionately interested in modern architecture.

I am now in my late 90s, an avid user of the internet and enjoying the power of computing, I am too old alas to keep up with new publications but I can still appreciate, from the sidelines, the enormous expansion of scientific knowledge and mourn the fact that it is not being made full use of to ensure the future viability of our planet and civilization.

AWARDS AND PRIZES

James Fraser, joint winner of the inaugural W. H. and W. L. Bragg Prize



The **2020 W. H. and W. L. Bragg Prize** for outstanding **early-career** crystallographers has been jointly awarded to James Fraser (Associate Professor in the Department of Bioengineering and Therapeutic Sciences at the University of California San Francisco, USA) and Jean-Philippe Julien [Senior Scientist at the Hospital for Sick Children (SickKids) and Associate Professor in the Departments of Biochemistry and Immunology at the University of Toronto, Canada] *as a recognition of their scholarly achievements as well as their strong commitment to serve the crystallographic community.*

The prize, which was established in 2017, celebrates the characters of the two Braggs, who actively encouraged young scientists, both women and men without discrimination, to pursue a career in crystallography. Their encouragement resulted in many young crystallographers achieving considerable distinction, including the Nobel Prize winners Dorothy Hodgkin, Max Perutz, John Kendrew, Francis Crick and James Watson.

Dr Fraser's research activities have been and are focused on studying the flexibility and conformational variability in macromolecules through experimental and computational methods. His research has provided new insights into how we can understand the role of protein flexibility in function through the use of crystallographic data. He has made seminal contributions to advancing the analysis of diffraction data in new directions, including the analysis of room-

temperature and temperature-dependent data to gain insights into protein dynamics, studies of diffuse scattering from proteins, and the development of new experiments to exploit X-ray free-electron lasers in this field. The two main developments, room-temperature X-ray data collection and structural ensemble modeling into weak electron density, contributed synergistically to help reveal the structural basis of protein dynamics, moving away from static representations towards more realistic descriptions of how proteins populate conformational space. Dr Fraser's innovative approaches contributed to translating fundamental discoveries in protein dynamics into improvement of protein engineering and drug design.

Drs Fraser and Julien will receive their award during the 25th IUCr Congress in Prague, Czech Republic, in August 2021, where they will share the presentation of a Keynote Lecture.

The IUCr was pleased to be able to conduct interviews with the winners about their life and work. Read the interview with James Fraser below and that with Jean-Philippe Julien [here](#).

INTERVIEW

James, we would first like to congratulate you on winning this prestigious award.

Could you tell us a little about your childhood and early education.

I was born in Toronto (literally across the street from where Jean-Philippe works now!) and attended fantastic public schools my entire life. My mother was a teacher and my father was a civil servant in the Ontario provincial government. Growing up I was obsessed with sports and especially the statistics in baseball and hockey.

What or who inspired you to pursue a career in science, and what attracted you to your field?

By the middle of high school, I wasn't really interested in science as something to study beyond high school. Although I had always done well in math and science, I never really was that excited about it. That all changed when I got to do some hands-on molecular biology thanks to a great teacher, Angela Vavitsas, who was able to get us access to some simple stuff like restriction enzymes and gel electrophoresis in our high-school biology lab. I got hooked by both the conceptual and mechanical (pipetting, *etc.*) aspects of it and haven't looked back.

Of which of your professional achievements do you feel most proud?

Although I'm proud of everything we have done in the lab, recently I'm most proud of the work a postdoc, Mike Thompson, has done getting time-resolved temperature jump experiments to work. The idea is what if we could nearly instantaneously heat the solvent that surrounds the protein and watch as the protein equilibrates to the new effective temperature. Mike got this working by SAXS (Thompson *et al.*, *Nature Chemistry*, 2019) and will publish some initial results by diffraction later this year. The diffraction work is awesome because it is the rare time you get to fire not one, but two lasers at something!

What would fascinate the Braggs about your work?

I think they would be interested in the theme of finding data in the imperfections of crystallography. I think the amazing thing about biomolecular crystallography is how even with great crystals, we still do a poor job of modeling the underlying data - what my friend James Holton calls "the *R*-factor gap". I've been fascinated by the problems of weak density in electron density maps and weak non-Bragg scatter on diffraction images for a long time. There is a lot of exciting work left to be done.

Currently, cryo-EM and X-ray crystallography are complementary approaches to structural biology and drug discovery. Do you see this changing in the future?

Yes, undoubtedly it will change. Right now the throughput of crystallography, especially for drug discovery, is unparalleled. But, there are paths for EM to catch up even in that respect eventually. The exciting things for crystallography are to do the things that EM can't do. Ultra-high resolution studies on small proteins. Fast dynamics. I see more and more labs (including my own) becoming agnostic to the method and focusing more on the common modeling challenges.

Since you were nominated for this prize, the world has been devastated by the coronavirus pandemic. Have you channelled any of your work into coronavirus research/education?

Yes, I've become part of a large effort, spearheaded by Nevan Krogan, here at UCSF to characterize the host interactome. Nevan's group identified hundreds of human proteins that are "hijacked" by SARS-CoV-2 proteins. There are two next phases that interact, identifying small molecules that can break those interactions and structurally characterizing the interfaces. Members of my group are working on both aspects as part of the UCSF QBI Coronavirus Research Consortium. I'm also optimistic that the sharing of data (for example the inspiring M^{pro} work out of Diamond Light Source) and increased use of preprints will help change the culture of science to prioritize more open and equitable practices.

You run your own lab. In a nutshell, what is your philosophy behind maintaining a happy and productive lab and mentoring its members?

I think I've improved a lot as a mentor by trying to keep my focus on where people in the lab are going next in their career. When we align our scientific goals with their career goals beyond my lab, we can do the best work together. Both the science and the career ambitions naturally change - and being open and communicative with each other about what we desire and what is realistic is the hard work of mentoring.



What are you seeking to accomplish in your career?

I don't know that this question drives me as much as it used to! Right now I'm interested in continuing to do the science that I find interesting and making sure that the folks who pass through my lab have a great time while they are there and are set on a great track. I've really enjoyed seeing how ideas that started in my lab have blossomed as trainees have moved on to their own positions in academia and industry. A major goal of mine is to reshape the way we communicate our science - I'd like to see us move to completely open lab notebooks and away from "saving" stuff for journal articles.

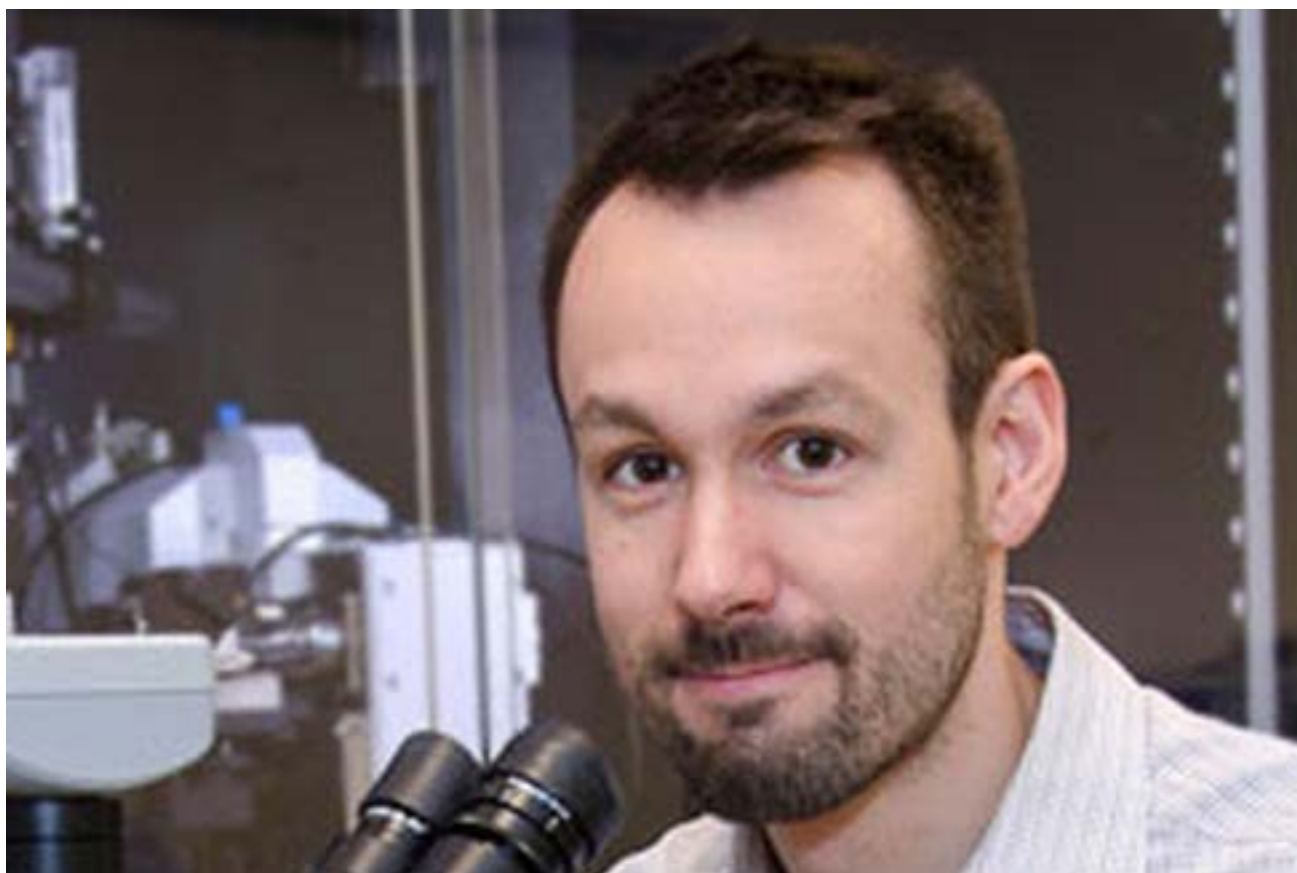
What other interests do you pursue?

Parenting! I have two young sons, who I spend most of my non-work hours chasing around. The shelter-in-place period of the recent pandemic has put a major emphasis on that!

Thank you very much for your time and congratulations once again

AWARDS AND PRIZES

Jean-Philippe Julien, joint winner of the inaugural W. H. and W. L. Bragg Prize



The **2020 W. H. and W. L. Bragg Prize** for outstanding **early-career** crystallographers has been jointly awarded to James Fraser (Associate Professor in the Department of Bioengineering and Therapeutic Sciences at the University of California San Francisco, USA) and Jean-Philippe Julien [Senior Scientist at the Hospital for Sick Children (SickKids) and Associate Professor in the Departments of Biochemistry and Immunology at the University of Toronto, Canada] *as a recognition of their scholarly achievements as well as their strong commitment to serve the crystallographic community.*

The prize, which was established in 2017, celebrates the characters of the two Braggs, who actively encouraged young scientists, both women and men without discrimination, to pursue a career in crystallography. Their encouragement resulted in many young crystallographers achieving considerable distinction, including the Nobel Prize winners Dorothy Hodgkin, Max Perutz, John Kendrew, Francis Crick and James Watson.

Dr Julien's research activities have been focused on the determination of crystal structures of macromolecules of high medical relevance. His studies have made a huge impact on biological and medical sciences. In particular, he determined the first crystal structure of an intact HIV envelope trimer by X-ray crystallography as well as by cryo-EM. The insights gathered from this structure and the construct engineering now serve as the template in the worldwide community for HIV

structure-based drug and vaccine design in the quest to curtail the HIV epidemic. Dr Julien has also determined the EM structure of a quaternary preferring antibody (PG9) in complex with the soluble SOSIP Env trimer. This work provided the first structural evidence that epitopes of broadly neutralizing antibodies are much more complex than thought. In this sense the corresponding publication in *PNAS* must be considered a paradigm-shifting publication. At present, Dr Julien's independent research programme is focused on two major areas: (a) structure-based immunogen design for the development of an anti-malarial vaccine, and (b) structural delineation of B-cell receptors. With respect to the latter, he embarked on a completely new direction of structural investigation of B-cell co-receptors, on nanoparticles engineered to target these receptors, and on characterising antibody responses to malaria antigens to aid in vaccine design.

Drs Fraser and Julien will receive their award during the 25th IUCr Congress in Prague, Czech Republic, in August 2021, where they will share the presentation of a Keynote Lecture.

The IUCr was pleased to be able to conduct interviews with the winners about their life and work. Read the interview with Jean-Philippe Julien below and that with James Fraser [here](#).

INTERVIEW

Jean-Philippe, we would like to first congratulate you on winning this prestigious award.

Could you tell us a little about your childhood and early education.

I am originally from Baie-Comeau, a small town in North-Eastern Québec, Canada. This name might ring a bell to fellow Canadians, as it's the small town where a former Canadian Prime Minister is from. I remember when I was young, that was our claim to fame for a small town otherwise little known by the outside world! After high school, I moved to British Columbia, Canada, to study at the Lester B. Pearson United World College of the Pacific. This College is unique in that it brings together 200 academically minded students from 50+ countries in a remote community. This educational experience allowed me at a young age to expand my perspective of the world and further appreciate its richness and diversity.

What or who inspired you to pursue a career in science, and what attracted you to your field?

I think scientists are curious people, and science is a great path for satisfying your utmost curiosity. It takes a lot of perseverance, optimism and creativity (and a bit of stubbornness!), because a lot of what we try on a daily basis will not work. I think those traits describe me pretty well, and so my personality aligns well with the scientific enterprise. I have also always looked up to scientists in history who, at one point or another, combined scientific creativity with social involvement. That has also been a major inspiration for my career.

Of which of your professional achievements do you feel most proud? What would fascinate the Braggs about your work?

Being part of interdisciplinary teams that succeed in surmounting scientific hurdles represent some of my deepest scientific satisfactions. During my post-doctoral work, I participated in such a team effort for the first structural determination of the pre-fusion HIV Env trimer led by my then post-doctoral supervisor Ian Wilson and our close collaborators. Now in my own laboratory, I have

the privilege of working with world-leading experts in immunology, pathogenesis, protein engineering, immunotherapy and many other experts in their respective fields. Science is truly multidisciplinary, and structural biology plays a central part in enabling discoveries and breakthroughs.

Currently, cryo-EM and X-ray crystallography are complementary approaches to structural biology and drug discovery. Do you see this changing in the future?

The cryo-EM resolution revolution has drastically changed the landscape of structural biology over the last decade. This technique, together with the high-throughput advantages of X-ray crystallography, can really deliver deep insights into molecular architectures of life when used in combination. In my opinion, the next frontier of structural biology will be the techniques that enable visualization of molecular machines directly in their natural environments.

Since you were nominated for this prize, the world has been devastated by the coronavirus pandemic. Have you channelled any of your work into coronavirus research/education?

Yes, our infrastructure and team know-how are currently being deployed in the response against SARS-CoV-2, in several projects. The pace of global scientific discoveries and open-access science has been truly remarkable. It is truly inspiring and humbling to be involved in such a transformative scientific wave. During this process, it has also been important to be active in graduate teaching on new technologies being deployed against COVID-19, as well as communicating regularly with the public in the media to provide scientific insights into discoveries being made and ongoing efforts to resolve unanswered questions.

You run your own lab. In a nutshell, what is your philosophy behind maintaining a happy and productive lab and mentoring its members?

I believe that everyone's work in my lab is driven in some shape or form by them wanting to make a difference. The best mentorship that I've received, and that I now try to perpetuate is the kind that connects with this drive, and cultivates it to grow.

What are you seeking to accomplish in your career?

Ultimately, I will be happy with my career if I can look back and find concrete examples of how I've helped make the world a better place. This can be in the form of inspiring trainees, providing critical guidance to young scientists, creating a new vaccine and/or drugs based on hypotheses derived from molecular blueprints, or influencing policies based on scientific data. In this context, I am driven most by the aspiration of bringing transformative technologies and knowledge to people most in need.

What other interests do you pursue?

Scientific discovery is a long journey, which most often shapes up more like a life-long marathon than a sprint! For this reason, I believe that finding a good life balance is critical. As best I can, I try to share the ups-and-downs of family life with my wife and our two sons, as well as stay active mostly by playing as much hockey as I can. After all, I am Canadian!

Thank you very much for your time and congratulations once again

AWARDS AND PRIZES

Sven Hovmöller, joint winner of the 2020 Gjønnnes Medal



Sven Hovmöller, Photo credit: Fredrik Persson/TT.

The **IUCr Gjønnnes Medal in Electron Crystallography** has been awarded to Sven Hovmöller (left; Professor Emeritus, Stockholm University, Sweden) and Ute Kolb (Head, Centre for High Resolution Electron Microscopy, Johannes Gutenberg-Universität, Mainz, Germany) *for their pioneering work in the field of electron crystallography, particularly for developing 3D electron diffraction techniques.*

In the 1990s, Sven Hovmöller and his group combined high-resolution transmission electron microscopy (HRTEM) images and zone-axis electron diffraction patterns for the solution of atomic structures. In 2007, Ute Kolb and her group developed the automated electron diffraction tomography (ADT) method, which allows the collection of 3D electron diffraction data suitable for structure analysis. As a result, atomic structures of many organic and inorganic crystals were solved. In 2008, Sven Hovmöller and his group suggested an alternative approach to collecting the 3D electron diffraction data – the Rotation Electron Diffraction (RED) method – which is also successfully used for the structure solution of complex structures, including proteins. Today, these methods are widely used by crystallographers all over the globe for the structure solution of new materials.

In addition to their outstanding scientific results, which were published in high-ranking international journals (*e.g. Nature and Science*), both scientists have been very active as organisers

of international schools on electron crystallography over many years. Thus, they have had a crucial role in the formation of a generation of electron crystallographers.

Professors Hovmöller and Kolb will receive their award during the 25th IUCr Congress in Prague, Czech Republic, in August 2021, where they will share the presentation of a Keynote Lecture.

The IUCr was pleased to be able to conduct interviews with the recipients about their life and work. The interview with Sven Hovmöller is reproduced below; please go [here](#) for that with Ute Kolb.

INTERVIEW

Sven, we would like to congratulate you on winning this prestigious award.

Thank you! Except for a poster prize once, this is my first scientific award, so I am very pleased.

Could you tell us a little about your childhood and early education?

I was born in Sweden but as a Danish citizen because my parents had just moved here from Denmark. My father was a meteorologist and as such he worked abroad for year-long positions several times. When I was 12 years old, he worked at the WMO (think WHO but for meteorology) and the whole family spent a full year in Geneva, Switzerland. This was in 1959, before charter tourism had become common, and I had the great pleasure to stay in this very beautiful and exotic country! Perhaps the best was that I went to Ecolint (The International School) in Geneva, in a class with pupils from all over the world: Italy, Egypt, Australia, USA, Sweden, Thailand, Indonesia That made me decide I should work with something where I could work in different countries.

What or who inspired you to pursue a career in science?

When I was 14, I started having chemistry as a subject at school and I immediately decided to become a chemist. And I stuck to that dream, something I never regretted, although I later understood that there are numerous other fields of science that are also extremely fascinating. To mention just a few: astronomy with exoplanets, comparative linguistics combined with DNA sequencing as a way to understand how all humans are related and how we migrated all the time.

Originally, I wanted to become a biochemist. For a number of reasons, I had to change subject, department and even university three times and supervisor six (!) times, before I finally took my PhD exam in crystallography, in 1980. Two of my supervisors got new jobs, two got the Nobel Prize (Aaron Klug in Chemistry and Bengt Samuelsson in Medicine, both 1982) and one (Samuelsson) sacked me.

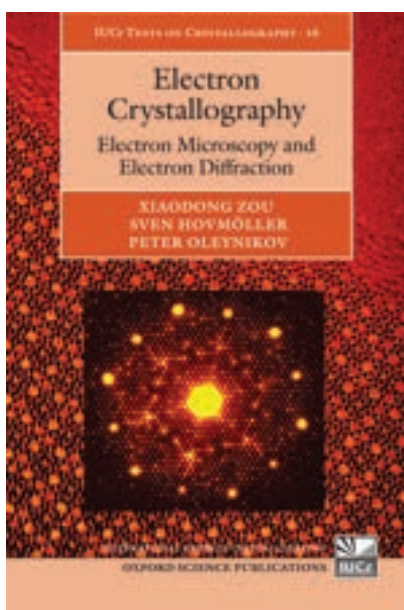
After repeatedly changing supervisor, I decided to finally study in a field where I could combine my interests in chemistry, computing and statistics (number crunching). I asked around and one day someone recommended crystallography. I had never heard of such a topic, but I tried it and I loved it.

When I was a child, my father would always demand the whole family to shut up during the weather report on the radio, which more often than not coincided with dinner time! He had decided, at the age of 8, to become a meteorologist. I always thought his main interest in life was the weather. But when he was over 90, he confessed to me that he wasn't really interested in the weather at all! He was just interested in all the numbers! As a young boy, he had first seen the

exchange rates in their local newspaper; so many numbers, and new numbers every day! At that point, he could have become a banker and the whole family would have become rich. But luckily, he soon found out that the local weather reports contained even more numbers, and so he decided to become a meteorologist. Now that I am 72 and have retired, I can honestly say that I never was very interested in chemistry, BUT THE NUMBERS! I loved them and I still love to look through tables with thousands of lines and dozens of columns, such as you can get in crystallography. And knowing that there are unknown scientific rules and principles hidden inside these numbers – yours to find out if you can just decipher the numbers!

And what attracted you to electron crystallography?

My very first PhD project was in biochemistry, trying to understand the mechanism of the ATPase of the mitochondria. At that time, 1969, almost nothing was known in this field. It wasn't yet established how many polypeptides formed the ATPase complex, and even less the molecular weight or even the sequence of these polypeptides. When I started my PhD studies in structural chemistry (crystallography) in 1973, I wanted to determine the crystal structure of the ATPase. My supervisor told me that was too hard for a PhD project, so he had me learn the basics in crystallography by determining single-crystal structures of a number of small organic molecules, related to DDT. In 1973, there were a few hundred crystal structures of water-soluble proteins, but not a single membrane protein was solved. It wasn't even clear what a membrane was. And then came the electron microscopy study by Nigel Unwin and Richard Henderson in Cambridge on the structure of bacteriorhodopsin! Like many others, I thought it might never be possible to make 3D crystals of membrane proteins. Many had tried, but nobody had yet succeeded. So I wrote to their boss, Aaron Klug, and asked to be accepted as a post- or predoc to work on bacteriorhodopsin. The positive reply said they didn't need more crystallographers on that project at the moment, but I was welcome to work on the structure of TMV (tobacco mosaic virus) and its specific binding to RNA. I was already familiar with the work of Klug on EM studies of viruses, tRNA *etc.* so of course I was more than delighted to come to work with Aaron Klug. I shared an office with Richard Henderson and eight others, so I got to know a lot also about membrane protein research.



After finishing my predoc and my PhD in 1980, I set up electron crystallography research in my own lab at Stockholm University, following the principles worked out in Cambridge. Later I

developed *CRISP* and other programs for electron crystallography, based on the Cambridge system but much more user-friendly and faster. I thought it would be necessary to make it easy to learn and use electron crystallography, if this method would ever become spread within new fields of chemistry and physics.

What are the advantages and limitations of electron crystallography when compared with X-ray crystallography?

The main advantage is that the much stronger interaction of electrons with matter makes it possible to study crystals a million times smaller than those needed for X-ray crystallography. Recently, we have shown that with modern computer-controlled electron microscopes and very fast and low-noise electron detectors, it is also possible to collect complete 3D electron diffraction data in just seconds, *i.e.* much faster than on the most powerful synchrotrons. Another advantage is that unlike X-rays, electrons can be focused into an image. In crystallographic terminology: we can observe experimentally not only the amplitudes (as in diffraction) but also the crystallographic structure factor phases.

Does electron crystallography have a special role to play in coronavirus research and other global problems?

I think most people on the planet see the same background illustration on the television news every day: a coronavirus particle. This is in fact an electron crystallography image, or rather the result of a 3D reconstruction from several EM images of the virus particle. It is today much faster to obtain a 3D structure of huge biological objects, such as viruses, by electrons than by X-rays. The last decade has seen the resolution in electron crystallography reaching beyond 2–3 Å, making it possible to get density maps so detailed that the polypeptide chain can be traced. Obviously, to have a 3D picture of the object you study is a great advantage when you want to plan a strategy for making a vaccine, or you want to understand the mechanism of the virus, in atomic detail.

You and Ute have been members of the IUCr Commission on Electron Crystallography (formerly IUCr Commission on Electron Diffraction). What would you say is the Commission's most important function?

- Educate next-generation electron crystallographers by arranging schools in electron crystallography
- Promote sessions in electron crystallography at crystallography conferences
- Encourage international collaboration within the fast-growing community of electron crystallographers
- Arrange visits by PhD students and scientists to each other's labs
- Make sure the methods developed in the various labs become user-friendly and available to the entire community, with X-ray crystallography as a role model.

You have been commended for your role in raising a generation of electron crystallographers through your international schools, many of which have been supported by the IUCr. With the necessary transition to online meetings in 2020, how do you see the future for face-to-face schools?

Nothing beats personal face-to-face interaction. Sometimes even a short conversation with an established person in your field can change the course of life for a young student.

This question also touches on a dark chapter of electron crystallography. I would like to take this opportunity to tell especially young scientists about it. It all started half a century ago.

During the 1960s, Aaron Klug developed optical diffraction of EM images of crystallographic samples. If you shine a laser on a periodic object, you will see a pattern of diffraction spots. You can try this at home: use a laser pointer and shine the laser light through any piece of textile. What you see is actually the Fourier transform of the image. At that time, there were no computers powerful enough to calculate Fourier transforms. Even 10 years later, in 1979, the calculation of a 256 x 256 Fourier transform was an overnight job at the mainframe computer at Cambridge University. Already in 1971 Klug wrote “The methods are closely analogous to those used by X-ray crystallographers to measure periodicities or degrees of order and finally to see the arrangement of atoms in simpler substances. The difference, however, is that there is no phase problem here because the phase information is contained in the electron micrograph” [*Phil. Trans. Roy. Soc. Lond. B* **261**, 173–179 (1971). III. Applications of image analysis techniques in electron microscopy. Optical diffraction and filtering and three-dimensional reconstructions from electron micrographs]. Clearly, Aaron Klug understood this fundamental difference between X-ray diffraction and EM images, already half a century ago, and he received the Nobel Prize in Chemistry in 1982 partly for this. Yet, a large part of the community in physical sciences working on EM was not aware of this. I tried for decades to spread the insights of Klug, as well as the spectacular EM work on membrane protein crystals by Unwin and Henderson, to everybody but with little success.

The scientific community working on EM images of inorganic compounds, such as minerals, semiconductors *etc.* always claimed that “the phase information is lost in images”. I, quoting Aaron Klug, claimed that “the phase information is present in images”. Any crystallographer will understand the magnitude of a disagreement on this point. When the IUCr in 1993 arranged a Summer School on Electron Crystallography at Tsinghua University, I wasn’t invited. I had taken the effort to fly to Arizona to introduce image processing by Fourier techniques to John Cowley, the honorary chair of this School. Cowley is considered as the father of electron diffraction physics. He stopped me when I said “and then we calculate the Fourier transform of the EM image, and at each diffraction spot we can now directly read out the phases”. “Wait a minute, let me think.” And then after a short moment, “Yes, you are right, please continue”. Obviously, Cowley was impressed by the demonstration and said “You know, next summer there will be an IUCr summer school on electron crystallography. I think you should go there to lecture. Would you be interested?” I was of course exhilarated and said yes. To be honest, my whole trip to Arizona was done only for the chance of hearing those words. Cowley wrote to the other dozen or so invited speakers to ask if I could be added to the list but got the majority vote NO. But I could come to give a computer lab. When I came to the school, there were no computers, no room for computers and no time allocated in the program for my computer lab. Luckily, my then PhD student Xiaodong Zou was also at the school. She immediately rented bikes for us and we cycled to the nearest shop and rented a couple of computers and huge displays. We could then stand in the corridor and run our lab in the coffee breaks.



Electron Crystallography School 1997 in Erice.

The school was then repeated in Bristol in 1994. Two members of the IUCr Commission on Electron Diffraction (as it was then called), Douglas Dorset and Boris Zvyagin, both pioneers of electron crystallography, suggested I should be invited as a lecturer to the Bristol school. The matter was discussed but after one member said “Hovmöller should not be invited because he confuses the students”, I wasn’t invited to that school either. This time I didn’t attempt to sneak in through the back door as I had done in Beijing. Instead I agreed with Xiaodong that we should just arrange our own schools. We then arranged a school at Stockholm University, with the students living in student dormitories and the conference dinner in our home with Xiaodong and her daughter Anna (4 years old) singing traditional Swedish Lucia songs. It was a success. Soon after, people who hadn’t been able to come asked for the next school. We had only planned to have one single event but it became one school after the other, first twice per year and then annually. After about 10 schools, we realized we were becoming something like Ludovico Riva de Sanseverino, who spent half his life arranging the IUCr schools in Erice. We then announced that we didn’t have any patent on making electron crystallography schools but we in fact would welcome any initiative to arrange schools in other countries as well. We would of course be happy to provide lectures, lecture notes, labs and suggest speakers, but the local organisers should arrange the hotels, meals and lecture rooms. This went very well, and by now these schools have been arranged in a dozen cities, most of them in Europe, but some occasional ones in USA, Korea and China. Gradually, local organisers, including Ute Kolb, took over all the duties. A very special highlight was when we managed to convince Ludovico to arrange one of our schools in Erice in 1997! From then it has become a tradition to have this Erice school every seven years (held in 2004, 2011, 2018, the next one in 2025).

How important is the recent initiative by the European Crystallographic Association and other organisations to provide childcare facilities during their meetings?

That’s a very good initiative. My first international conference was in 1973, and then the social program was still called “Ladies program”. At the International Zeolite Conference in Montpellier in 2000, my wife, Xiaodong Zou, had already overtaken me in terms of scientific career so I accompanied her to the conference, looking after our new-born, Linus, so Xiaodong could keep

breast-feeding Linus and I could take part in the “Ladies program” (which by that time actually was called Social program in every conference).

What other interests do you pursue?

I am mainly involved in political and social issues since I retired six years ago. I have started a “Chemistry Club” mainly for exceptionally gifted children, aged 5–12. We give lectures at the university level for these kids, and get hundreds of questions during a two-hour lecture. Most lectures are on chemistry, but some are about physics, mathematics or biology. One evening I presented in three Asian languages: Chinese, Japanese and Korean. However, they only had to learn to read Korean in those two hours.

At the other end of the spectrum, I chair a small organization helping Romanian beggars in Sweden to find shelter, learn to write their first name and later to speak and read Swedish, to find a job *etc.* The European Roma are among the poorest and most discriminated people on Earth. Even today, millions have not attended school for a single day, and hardly any more than eight years.

Of which of your professional achievements do you feel most proud?

I am proud and content that, with others, we have managed to develop electron crystallography from a small field into a mainstream method. In the last decade, we have gone from a very time-consuming (years) and demanding field for 2D projections only to ultra-fast (minutes) 3D structure determination of very complex structures, including proteins. In fields such as zeolites, metal-organic frameworks and pharmaceuticals, important structures that have remained unknown for up to 100 years have now been solved by electron crystallography. Typically, they form crystals too small for single-crystal X-ray crystallography and too complex for X-ray powder diffraction. Some are multiphasic and/or full of defects. For electrons, even the smallest powder particles are single crystals.



Sven Hovmöller and his son, Linus Hovmöller Zou, solving the crystal structure of PD quasicrystal approximants.

What has made me most happy and proud was when our then 9-year old son, Linus, in 2010 solved a set of very complex quasicrystal approximants, called pseudodecagonal (PD1, PD2 *etc.*).

They are made synthetically in alloys of composition $\sim\text{Al}_{70}\text{Ni}_x\text{Co}_{30-x}$. Together with three collaborators, I had spent half a year full-time trying to solve these structures but with no success. Every summer for about eight years, I had more and more desperately tried to solve them, but no. We had hundreds of HRTEM images and electron diffraction patterns, but the structures resisted being solved. Then in 2010, I gave it a try again and got stuck. It was during the summer vacation and Linus was around at home. I asked him “Linus can you come here for a while and help your dad?” He sat down at our huge kitchen table, full of diffraction patterns, EM images and computers. Linus is very clever at pattern recognition and his head was not as completely muddled as mine from looking at and remembering hundreds of these images. So he could object to my suggestions and after a full 8-hour day, we had solved the first two PD structures! We continued the following day and finally managed to solve in total four of these very complex structures. We decided to have Linus included as one of the co-authors, given his critical contribution to finally solving these structures. I told the editor that one of the authors, Linus Hovmöller Zou, was only 9 years old. It took a year before it was published and then the editor informed me and also wrote “We mentioned in the press release that one author is only 9 years old.” And then RING! The phone was on fire, with calls from the BBC, *The Times* and many Swedish and international newspapers. They got interviews with Linus, in English. We were on television. You can still see the BBC reportage by Googling BBC Linus Hovmöller Zou. As it turns out, Linus is the youngest boy ever to co-author a scientific paper. Only an American girl was a few months younger.

Thank you very much for your time and congratulations once again.

Thank you!

AWARDS AND PRIZES

Ute Kolb, joint winner of the 2020 Gjønnnes Medal



Ute Kolb speaking at the Electron Crystallography School 2011 in Erice. Photo credit: Peter Müller.

The **IUCr Gjønnnes Medal in Electron Crystallography** has been awarded to Sven Hovmöller (Professor Emeritus, Stockholm University, Sweden) and Ute Kolb (Head, Centre for High Resolution Electron Microscopy, Johannes Gutenberg-Universität, Mainz, Germany) *for their pioneering work in the field of electron crystallography, particularly for developing 3D electron diffraction techniques.*

In the 1990s, Sven Hovmöller and his group combined high-resolution transmission electron microscopy (HRTEM) images and zone-axis electron diffraction patterns for the solution of atomic structures. In 2007, Ute Kolb and her group developed the automated electron diffraction tomography (ADT) method, which allows the collection of 3D electron diffraction data suitable for structure analysis. As a result, atomic structures of many organic and inorganic crystals were solved. In 2008, Sven Hovmöller and his group suggested an alternative approach to collecting the 3D electron diffraction data – the Rotation Electron Diffraction (RED) method – which is also successfully used for the structure solution of complex structures, including proteins. Today, these methods are widely used by crystallographers all over the globe for the structure solution of new materials.

In addition to their outstanding scientific results, which were published in high-ranking international journals (*e.g. Nature and Science*), both scientists have been very active as organisers of international schools on electron crystallography over many years. Thus, they have had a crucial role in the formation of a generation of electron crystallographers.

Professors Hovmöller and Kolb will receive their award during the 25th IUCr Congress in Prague, Czech Republic, in August 2021, where they will share the presentation of a Keynote Lecture.

The IUCr was pleased to be able to conduct interviews with the recipients about their life and work. The interview with Ute Kolb is reproduced below; please go [here](#) for that with Sven Hovmöller.

Interview

Ute, we would like to congratulate you on winning this prestigious award.

Thank you very much. I am extremely pleased that the crystallographic community is honoring my work and my achievements in electron crystallography.

Could you tell us a little about your childhood and early education.

I was born in 1963 and grew up in Bingen, Germany, a small town in the UNESCO World Heritage Site on the river Rhine. My father, an X-ray technician, and my mother, a medical-technical assistant, besides their normal jobs also did agriculture and ran a fish farm. My mother later stayed at home after the birth of my youngest sister. Even then, I was more interested in the technical processes in my father's workshop than in the housework – as expected at that time. Although I could learn a lot from my father in this way, I owe it to my mother that I was able to take my A levels. She actively supported me against the then-common view that "Girls don't need a high school diploma and should later only care for their family and children anyway". This support has given me the motivation to pursue my goals.

What or who inspired you to pursue a career in science?

I have always been interested in mathematical correlations and during my school days at the Hildegardis School, a Catholic grammar school for girls, I dreamed of becoming a teacher of mathematics and physics. However, just before the final choice of subject, I decided on chemistry as the less descriptive and more directly applied natural science in my eyes. I received great mental support for and during my studies from my then boyfriend and now husband, Norbert Bittner. He was also the one who encouraged me to apply for summer studies at CERN in Geneva. In my childhood, due to the agricultural orientation of my parents, trips abroad were extremely rare. Thus, my view of the world broadened abruptly with this first contact with international students and international research. Even though there wasn't the need for inspiring me to pursue in science, this experience with scientists from all over the world opened up my mind to the diversity and satisfaction that lies in it.

And what attracted you to electron crystallography?

During my studies, following my penchant for mathematics and physics, I focused on physical chemistry and graduated in this field. But it was not until I started my doctoral studies in the group of Martin Dräger in Inorganic Chemistry that I got to know the fascination of crystallography and its symmetries – by applying X-ray diffraction methods. When I decided to join Ingrid Voigt-Martin's

group as a postdoc after completing my PhD, I was motivated by the desire for a new challenge. The electron diffraction method used to acquire data in this group offered me the scope for development – by applying my knowledge of X-ray structure analysis to quantification of electron diffraction data, I was able to combine my passion for structure analysis with my love of crystallography. I was impressed by the unique feature of an electron microscope to obtain images and diffraction patterns of nanoscopic particles. And it was the stunning aesthetics of electron diffraction patterns that immediately captivated me. Even today, I still consider electron crystallography to be the most direct method of understanding or teaching diffraction physics. I learned the structural analysis of electron diffraction data during extremely instructive stays with Douglas Dorset in Buffalo and Chris Gilmore in Glasgow. For evaluation of zonal diffraction data we used the programs of Sven Hovmöller. However, the structural analysis of small organic molecules with data from conventional acquisition turned out to be extremely problematic and often only succeeded by combining it with other information. I soon realized that in order to solve structures not accessible by X-ray powder diffraction directly from electron diffraction data, I had to improve the acquisition of diffraction data considerably. When later, in 2007, the first *ab-initio* structural analysis of barite was performed, I did not yet realize that this would be the foundation for a widely applicable 3D electron diffraction method.

This success was made possible by a postdoctoral position of the state of Rhineland-Palatinate in 1997 for the development of an alternative method for crystal structure analysis by electron diffraction. I am especially grateful to Gertrude Kiel, who encouraged me to take this step as well as to Wolfgang Tremel who supervised my habilitation and supported me throughout my scientific career. With the acquisition of further funds, I was able to put together a small but very powerful working group. I would especially like to mention my first co-workers, Tatiana E. Gorelik and Enrico Mugnaioli, who were directly and significantly involved in the development of the methods.

What are the advantages and limitations of electron crystallography when compared with X-ray crystallography?

The fundamental difference between electron radiation and X-rays is their charge and the much stronger interaction with matter associated with it. For example, X-ray structural analysis requires crystals in the range of cubic micrometers, whereas electron diffraction requires only a scattering volume in the cubic nanometer range. In addition, light elements can be better detected with electron radiation. A unique feature is the possibility to switch directly between the projection of the potential (image) and its Fourier transformation (diffraction) in the transmission electron microscope as well as to determine the elemental composition of the particle by spectroscopic analysis. All data can be tomographically recorded separately or in combination. This allows, for example, to select individual crystallites from a phase mixture and collect 3D diffraction data for crystal structure analysis, or *vice versa*, to evaluate diffuse scattering patterns detected in the diffraction space and to correlate them with the imaging of defects in the particle. Compared with X-ray diffraction, more complex sample preparation is required, depending on the material and the problem. The strong interaction of electrons with matter requires the preparation of thin samples, which can lead to artifacts. In addition, the sample should be stable during the measurement in vacuum, in the electron beam and under cooling. *In-situ* investigations in the transmission electron microscope are intensively developed, but this type of experiment is more easily accessible in the case of X-ray diffraction. The acquisition of a 3D electron diffraction data set with conventional

CCDs takes about 10 min, which is further reduced by the use of new detector technologies. This not only gains time but also reduces the already low electron dose required for diffraction experiments compared with imaging methods even further. In addition to the technical and methodological development of transmission electron microscopes, the first dedicated electron diffractometers are already under development. The high complementarity of electron crystallography to X-ray diffraction, but especially to X-ray powder diffraction, suggests that in the future more and more electron diffractometers will be added to the equipment of laboratories and departments for structural elucidation.

Does electron crystallography have a special role to play in coronavirus research and other global problems?

Electron crystallography has already been used to image the coronavirus and, by elucidating the structure of its spikes with the help of 3D reconstructions, will certainly make further important contributions to the fight against the virus. Furthermore, electron crystallography is already involved in many projects to solve global problems. Scientists are using findings from electron crystallography, for example, to improve catalysis, energy storage, for alternative energies, in aerosol research, for CO₂ reduction, in the field of biomineralization, in the analysis of active ingredients for pharmaceutical purpose and in medical technology. In addition, many open questions in mineralogy or archaeology that had been open for decades have been solved.

You and Sven have both been members of the IUCr Commission on Electron Crystallography (formerly IUCr Commission on Electron Diffraction). What would you say is the Commission's most important function?

In my view, the Commissions of the IUCr have their key role in the worldwide networking of scientists, in improving the visibility of the respective field of interest and as a lobby for the scientific community. Networking is particularly important for electron crystallography, since all scientific disciplines that use electron scattering are represented here. However, the strong diversity also provides us the opportunity to learn from each other, to work together internationally and interdisciplinarily as well as ultimately to act together to promote the whole field of electron crystallography. The organization of pure sessions on electron crystallography or joint symposia and contributions at large conferences allow this interdisciplinary communication, while workshops enable a deeper and more concentrated exchange. Both are important. However, the training and networking of young scientists, first in schools and then in more in-depth workshops or through doctoral student exchanges, plays a special role, as this is where the foundation for future generations is laid.



Electron Crystallography School 2011 in Erice. Left (from left to right): Enrico Mugnaioli, Andrew Stewart, Iryna Andrusenko, Ute Kolb, Tatiana E. Gorelik, Sebastian Schlitt (photo credit Dr Peter Müller, MIT, Cambridge, MA, USA). Right: group photo.

You have been commended for your role in raising a generation of electron crystallographers through your international schools, many of which have been supported by the IUCr. With the necessary transition to online meetings in 2020, how do you see the future for face-to-face schools?

The benefits of international schools go far beyond the mere transfer of knowledge. The knowledge itself can easily be passed on through online sessions. What is missing, however, are the aspects that go beyond hard facts, such as personal conversations with teachers and fellow students, spontaneously arising debates on an open question or the experience of emotional moments. I still remember how deeply impressed I was by my encounter with Dorothy Crowfoot Hodgkin at the Nobel Laureate Conference in Lindau in 1989, or by my first visit to the Electron Crystallography School in Erice in 1997, and how at this occasion the world in my head expanded, similar to what happened in my summer studies at CERN. When I got the chance to lead the Electron Crystallography School 2011 in Erice together with Louisa Meshi and Anatoly Avilov, we made sure that all disciplines of electron crystallography were linked as much as possible and planned the school consciously parallel to a powder diffractometry school. Three years later, my simultaneous teaching activities at the Johannes Gutenberg University Mainz and at the Technical University Darmstadt enabled me to organize an electron crystallography school in Darmstadt. A special feature of the school was the extensive direct training facilities at both locations with transmission electron microscopes from different manufacturers and different levels of expansion. At both universities, I have taught for many years the basics of electron crystallography to students already in the main study period *via* lectures and practical courses. For the summer semester 2020 the lecture was held online. The practical course was realized with a specially made educational film and an online supervision *via* webcams from the neighboring room.

In my opinion, we will still need schools and workshops in the future as face-to-face events for the above-mentioned reasons. On the other hand, online meetings offer a much more efficient and less time-consuming way of communication – as concepts and platforms are further developed and improved, they might offer new formats and possibilities that supplement the traditional formats. However, nowadays we must take into account the existence of the coronavirus and develop new concepts that are offering the best possible experience and inspiration together with the highest possible security for all participants of these schools.



Electron Crystallography School 2014 in Darmstadt.

How important is the recent initiative by the European Crystallographic Association and other organisations to provide childcare facilities during their meetings?

For a scientist, attending a conference should not become a choice between family and career. Therefore, everything should be done to avoid this balancing act. Childcare is an important

measure but does not apply to infants. I still remember the IUCr meeting in Florence. My daughter Helena was just 5 months old and became the youngest participant of the conference with a badge issued especially for her. Fortunately, my husband was able to accompany me so that I was free to follow the presentations. Not only in Florence, but also at several other conferences he took part in the "Social Program", looked after our daughter and kept my back free for science. In case the use of the childcare facilities is not adequate, for example for young parents with infants, in my opinion the financial support of the IUCr for an accompanying person would be helpful, possibly even just by granting free access to the conference area.

What other interests do you pursue?

In my free time I prefer to devote myself to my family and activities that allow me to take a deep breath. These include outdoor activities such as climbing, cycling or hiking, but also music. In the time of my studies and my doctorate I could still take the liberty of participating in several choirs. Unfortunately, this is no longer the case. I take a lot of pleasure as well in design and live it out by sporadic work in the garden.

Of which of your professional achievements do you feel most proud?

It was a particularly proud moment when the first publication on the structural analysis of barite was printed in 2007. Ultimately, 10 years of gradual method development with many ups and downs were behind this publication. When I started working on electron diffraction, very few scientists were working on this topic and data acquisition was difficult and time-consuming.

During the following years my group was able to show on a variety of different compounds, such as minerals, zeolites, oxidic materials, metal-organic networks or small organic molecules like pharmaceuticals, that the use of 3D electron diffraction data taken from unoriented crystallites allows an *ab initio* structural analysis and proves the efficiency of the principle of automatic diffraction tomography (ADT). The community of electron crystallographers has grown rapidly since then. Today, many new developments are available, which differ both in the way the data is acquired and how it is processed, but all follow the same basic principle of electron tomography. The variety of methods offers the possibility to future generations of electron crystallographers to choose the optimal method for the respective material, the problem and the available equipment. In my group, for example, we prefer to use ADT in STEM mode coupled with electron beam precession, which allows us to image even very small and thin crystallites with sufficient contrast to track the crystal during tilt. I was especially proud of the solution of the long-time unknown crystal structure of vaterite on a 30 nm small crystallite in 2012 and the solution of a new hydrate phase of CaCO_3 in 2019, the calcium carbonate hemihydrate.

Many already existing transmission electron microscopes can be used directly or with some extension for 3D electron diffraction methods (3DED), thus being applicable for less well-equipped laboratories. In addition to the large centers, a broad international base of electron crystallography experts can thus be established, who are able to address the huge variety of crystallographic questions raised for the solution of existing and upcoming global problems.

Thank you very much for your time and congratulations once again.

In the course of time I met many fascinating people who impressed me in different ways, shaped me and made a great contribution to my scientific career. I would like to take this opportunity to

thank everyone who supported me on my not always straightforward path and made this moment possible.

AWARDS AND PRIZES

Aminoff Prize rewards “explosive” studies of biological macromolecules



From left: Henry Chapman, Janos Hajdu and John Spence, winners of the Gregori Aminoff Prize 2021.

The Royal Swedish Academy of Sciences has decided to award the [Gregori Aminoff Prize 2021](#) to Henry Chapman (University of Hamburg, Germany), Janos Hajdu (Uppsala University, Sweden) and John Spence (Arizona State University, Tempe, AZ, USA) “for their fundamental contributions to the development of X-ray free electron laser based structural biology”. The Prize rewards a documented individual contribution to the field of crystallography, and has been awarded to Swedish and foreign researchers since 1979.

Professors Chapman, Hajdu and Spence (shown from left to right) are pioneers in the development and application of X-ray free-electron lasers (XFELs) in the study of biological macromolecules, especially proteins. Thanks to the intense X-rays generated in a single short pulse from an XFEL, the structure of highly sensitive protein samples can be obtained using an experimental approach called “diffraction before destruction”, where diffraction data are generated and recorded before the crystal explodes. This has now been done for various proteins that function as surface receptors on human cells, opening the way for new pharmaceuticals to be developed.

The short pulses from an XFEL also allow the study of extremely rapid reactions that are catalysed by proteins and radiation-sensitive reactions. An example is the key enzyme in photosynthesis, photosystem II, where XFEL research allows the structure determination of intermediate molecules, ones that are created and changed during the reaction. This, for example, has improved the understanding of how atmospheric oxygen is generated from water in plants, in a reaction that provides energy for the fixation of atmospheric carbon dioxide.

All three winners are well known to IUCr Journals, with Professor Hajdu being Editor of *Journal of Applied Crystallography*, and Professors Chapman and Spence Co-Editor (Physics and FEL Science and Technology) and Editor, respectively, of **IUCrJ**.

For a list of papers by Henry Chapman appearing in IUCr journals click [here](#).

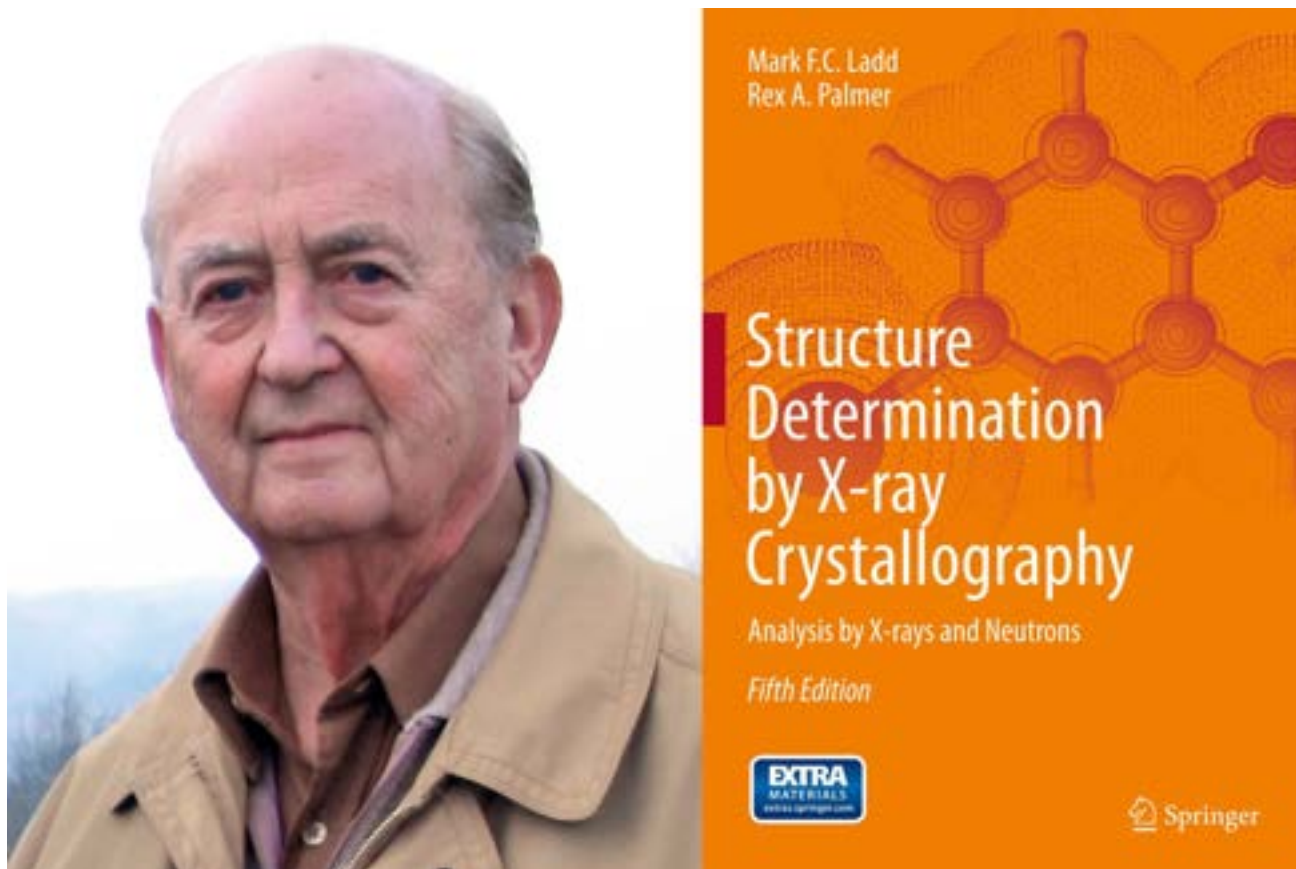
For a list of papers by Janos Hajdu appearing in IUCr journals click [here](#).

For a list of papers by John Spence appearing in IUCr journals click [here](#).

OBITUARY

Marcus Frederick Charles Ladd (1926-2020)

David Povey



Mark Ladd's long association with the University of Surrey, UK, goes back to the 1950s. As a young graduate, he was employed by GEC in their Hirst Research Centre in Wembley, travelling daily from Tottenham to Wembley on his trusty moped. One part of GEC was investigating the structural aspects of a range of materials considered to be of commercial interest to the company and Mark joined the X-ray crystallography group. Their remit was wide ranging and covered the development of a range of techniques to study the properties of a large range of polycrystalline and single-crystal materials and this is where his interest in the solid state and its characterisation began to evolve.

He may well have stayed at GEC had it not been for developments which were taking place in Higher Education. In 1956 the then Battersea Polytechnic, following a government White Paper, became one of the Colleges of Advanced Technology. In keeping with this advanced technology remit a new department was created "Chemical Physics and Spectroscopy" under the headship of Professor Victor Griffiths. "Griff" as he was always known was keen to recruit academic staff who had good experience of industry. It is not clear how "Griff" and Mark Ladd first met although "Griff" was well known for having a wide net of industrial contacts, but Mark always remembered his first meeting over a cup of tea in a café in Battersea Park Road. Soon after, he was on the teaching staff of the new CAT as a junior lecturer. The new department was situated in an annexe some distance away from the main college in an old school building in Falcon Road, Battersea, which resembled a rabbit warren. New staff were not given offices and the whole arrangement was very open plan.

“Griff” was always keen that his staff had the opportunity for postgraduate study and in 1958 Mark registered for a PhD at Birkbeck College on a part-time basis working on the crystal structure of euphenyl iodoacetate with Dr C. H. Carlisle as his supervisor. There was little X-ray diffraction equipment available at Falcon Road so most of the experimental work was carried out at Birkbeck College. In his spare time away from teaching duties, Mark would travel to Birkbeck to carry out the experimental work setting up multiple film packs on a Weissenberg camera. “This was hard work going back and forth to Birkbeck but fortunately the exposures often took a few days so I could leave them running with the technical staff at Birkbeck looking after them”. Later in his career he loved to explain to students the real labour of love to get a set of X-ray intensity data measured by eye with a calibrated film strip coupled with the necessary scaling from successive films.

In the early 1960s the college had purchased a new computer, an Elliot 503, and this to Mark’s delight was sited at Falcon Road. He taught himself ALGOL which was the only programming language available and was able to carry out some of the calculations required for his research. Unfortunately, the relatively small capacity of the machine and its lack of availability during the day meant that some of the long calculations had to be performed overnight. Three-dimensional electron density maps required intermediate summations to be output on punched paper tape which then had to be subsequently re-input and Mark had a camp bed installed so that he could keep track of all the calculations. His PhD was awarded in 1965.

Apart from his teaching duties in his own department, Mark was keen to interact with other departments at Battersea so when the head of chemistry asked if he would like to “do something on crystallography” for a final year physical chemistry course he jumped at the opportunity. “When I asked how many lectures I could have, back came the reply, “just one””. But he did it, it was done at a fast pace with a lot of detailed handouts but it also gave him the opportunity to advertise the new MSc course in crystallography which he was in the process of organising.

In 1968, the college was granted its royal charter and it moved to Guildford as the University of Surrey. The departmental name was changed to Chemical Physics, and Mark was charged with organising the layout of the department. “if it was going to be done, it had to be done properly. I remember going to see “Griff” with my requests for equipment. He would disappear to see someone he knew from industry and use his very persuasive powers to find either money or second-hand equipment”. The results of his efforts were fully equipped teaching and research laboratories with a complement of single-crystal cameras, powder diffractometers and a four-circle Siemens single-crystal diffractometer. In addition, there was a crystal optics laboratory and a well-resourced model room. The geographical position of Chemical Physics within the campus allowed the setting up of interactions with the departments of Metallurgy, Physics and Chemistry and the proximity of organisations such as the Royal Aircraft Establishment allowed the MSc course to be run on a part-time as well as a full-time basis.

As Head of Department and Reader in Chemical Crystallography Mark was always committed to chemical physics as a separate discipline and to this end, he made sure that all the undergraduate and taught postgraduate students had the opportunity to study mathematics, “proper maths” as he called it.

At this time, there was little or no opportunity to use computers to enhance lectures so all visual aid material was constructed by hand and he produced a large number of expertly drawn transparencies to explain the many aspects of crystal geometry and symmetry as well as producing a collection of some 300 35-mm photographic slides. Fancy automatic slide projectors did not exist or were too expensive, so he acquired an ancient slide projector which was brought along to his lectures.

The 1970s were a time of change. Personal computers were evolving, and Mark saw this as a real opportunity to enhance the chemical physics degree. Within this framework, he developed the concept of two distinct themes, the science of measurement and the science of structure. The former was based around the use of microcomputers as a means of monitoring and controlling a range of scientific

processes. The latter expanded the solid-state themes into studies of surface structure, electron diffraction and crystal growth in collaboration with the metallurgy department.

In 1981 the Higher Education sector in the UK suffered severe financial cutbacks. Several departments at Surrey were closed and Chemical Physics was subsumed into Chemistry as a sub-department although still retaining its independence and academic head. However this gave Mark the opportunity to form stronger links with the various synthetic chemistry groups which were further strengthened when he persuaded the university to purchase a new Enraf-Nonius CAD-4 diffractometer and he got great pleasure in persuading many PhD students in these groups to think about including structure determination of some of the molecules that they were synthesising.

However, as time progressed numbers of students on both the undergraduate chemical physics and taught masters course started to decline and eventually the university decided to close both courses. It was with great sadness that Mark agreed to this although he did persuade the chemistry department that some of the chemical physics modules would make ideal final-year options and he continued to contribute to these.

Over his long career Mark authored or co-authored many textbooks. The first of these, *Practical Radiochemistry*, was co-authored with W. H. Lee, a physical chemist working in the chemistry department at Battersea. This was the start over several years of a whole series of books covering physical chemistry, structure and bonding, symmetry in molecules and crystals, and structure determination by X-ray crystallography (with R. A. Palmer). Even after retirement he was insistent that the textbooks should be kept up to date. Many underwent subsequent revisions with new sets of problems and computer-based material which was made available on an accompanying website.

Outside of the university Mark was passionate about music. He played the double bass as a member of the Croydon Symphony Orchestra and also played the viola. Students undertaking some of the practical modelling classes which he supervised would find a classical melody playing quietly in the background as “relaxation” for them. None of the students dared ask whether they could have something a bit more modern!

He became interested in Doberman dogs after a friend gave them their first Doberman. This developed into showing the animal at Crufts where it won best in breed and was the start of more than a hobby. Mark moved into breeding Dobermans, importing animals from the USA and eventually producing a book on Doberman genetics. He was also president of the Surrey Doberman Society for several years. The first that anyone knew about the developing interest in dogs was when one was proudly brought into the department much to the anxiety of the departmental secretary, not a dog lover. Feeling that she had to say something she asked Mark what the name of the animal was. Mark with his usual attention to detail came out with the long Kennel Club registered name. “I shall never remember that said the secretary, the dog is brown in colour, I shall call him Mr Brown”. From that day on, everybody in the department, staff and students knew Mr Brown who used to sit quite happily in the corner of Mark’s office.

At the age of 80, and indicative of his adventurous spirit, he and his wife decided to swap the comfort of suburban Farnham to a more remote existence in Bramshott where he continued with his writing and he was often to be found in the chemistry department talking about some ideas about a new book he was planning.

Sadly, declining health curtailed many of his activities although he was still active in writing and his final book, *The Essence of Crystallography*, was published at the end of 2019.

He lost his beloved wife of 69 years, Val, only five weeks before he died and he leaves two sons, Tony, a Professor in the Chemical Engineering Department at the University of Florida, USA, and Nick, a Church of England Minister.

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OBITUARY

Marilyn M. Olmstead (1943-2020)

Christine M. Beavers



Marilyn Olmstead, Professor Emerita at UC Davis, CA, USA, pictured at the ACA2009 meeting in Toronto, ON, Canada (photo credit: W. L. Duax). Marilyn, who was a well-liked and highly valued Co-editor on *Acta Cryst. E* during the period 2000 to 2011, died in an accident while riding her bike near her home.

The person you knew would have the answers. The person who would help you analyse a challenging situation. The person who would recommend just the right outdoor activity to clear away that gloom. The person who gave you a home in science, encouraged you and convinced you that you belonged. That you mattered. Marilyn was all of those people, to me and many others.

It's a warm October day in the San Francisco bay area, two weeks to the day after I was awoken at 1am to receive the most tragic of news. The words at the time seemed hydrophobic and immiscible to my sleep-sodden mind - slipping and sliding across the surface of my consciousness, but not ever soaking in. Seeking solidarity in shock, I messaged a number of my academic siblings. Joined over the various apps that have recently become our social lifelines, we muttered the same phrases of disbelief. Struggling for words, we eventually ended our calls with promises to talk again soon. I then turned to social media and swiped through photos of happy times with Marilyn, until I couldn't see through the tears.

Over the past two weeks, the slow diffusion of acceptance has illuminated more facets of this devastating loss. Memories of past adventures together are now glazed with a somber patina. Future plans and projects glow with a diminished lustre, seemingly without hope of being blessed with Marilyn Magic. However, amongst all this grief, we humans continue to do the thing we do so well: weave our stories into a mourning tapestry, rich in memories and comfort. Marilyn's youth as a natural scientist,

examining lizards and becoming a ham radio operator at the age of 13. Marilyn's persistence and brilliance in academia, despite its hostility towards women. Marilyn's patience and kindness while mentoring. Pomegranate-jelly-making sessions perennially marking the arrival of autumn. Trips to Tahoe in the summer for hiking and swimming; trips to Tahoe in the winter for skiing and snowboarding. Marilyn's dedication to international collaborations, and her love of immersive travel, where she truly stretched herself to experience a culture while expanding her collaborative family. The whirlwind experience of being at a crystallography conference with Marilyn, and feeling like you are partying with a rockstar. Nearly all of these testimonials included hypothetical questions in the vein of "How will we go on without Marilyn?" I know I felt similarly; none of us feel ready to step into such colossal shoes. Another common thread within all these stories was the incredible amount of energy that Marilyn imbued into all her interactions. A dynamic energy when the tricky structure as well as a student's success were close at hand. A courageous energy that defied all limits and encouraged others to dream bigger. A compassionate energy when the challenges seemed insurmountable and emotion ran high.

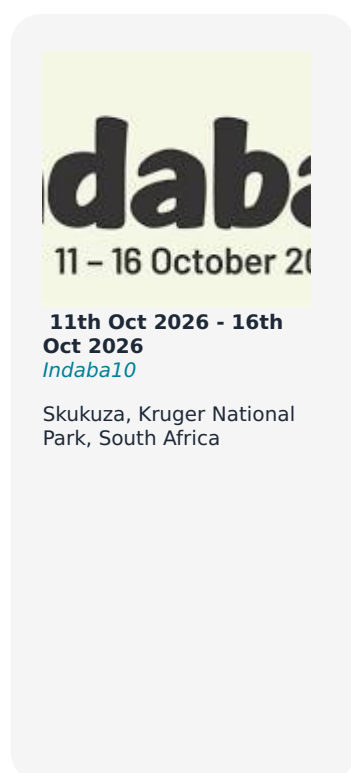
Through all these stories, we are reminded that Marilyn believed in us. She trusted us to take the tools she gave us and go forth. When our confidence flagged, she cheered us on. When we were unsure, she helped us determine the facts of the matter and weigh them appropriately. We are now faced with this grievous time, where we are without her counsel and cheer, and are feeling adrift in this loss. May we all follow Marilyn's encouragement, and see ourselves more as she saw us; going forward together, with courage and compassion, would certainly make her proud.

IUCr SUPPORTED EVENTS

IUCr supported meetings

During this period of meeting cancellations and postponements because of international health concerns, the IUCr will make best efforts to indicate the status of advertised meetings whenever we receive updates. Please refer in all cases to any website maintained by the meeting organizers for definitive information.

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





5th Dec 2026 - 10th Dec 2026

African Materials Research Society (AMRS 2026)

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

During this period of meeting cancellations and postponements because of international health concerns, the IUCr will make best efforts to indicate the status of advertised meetings whenever we receive updates. Please refer in all cases to any website maintained by the meeting organizers for definitive information.

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