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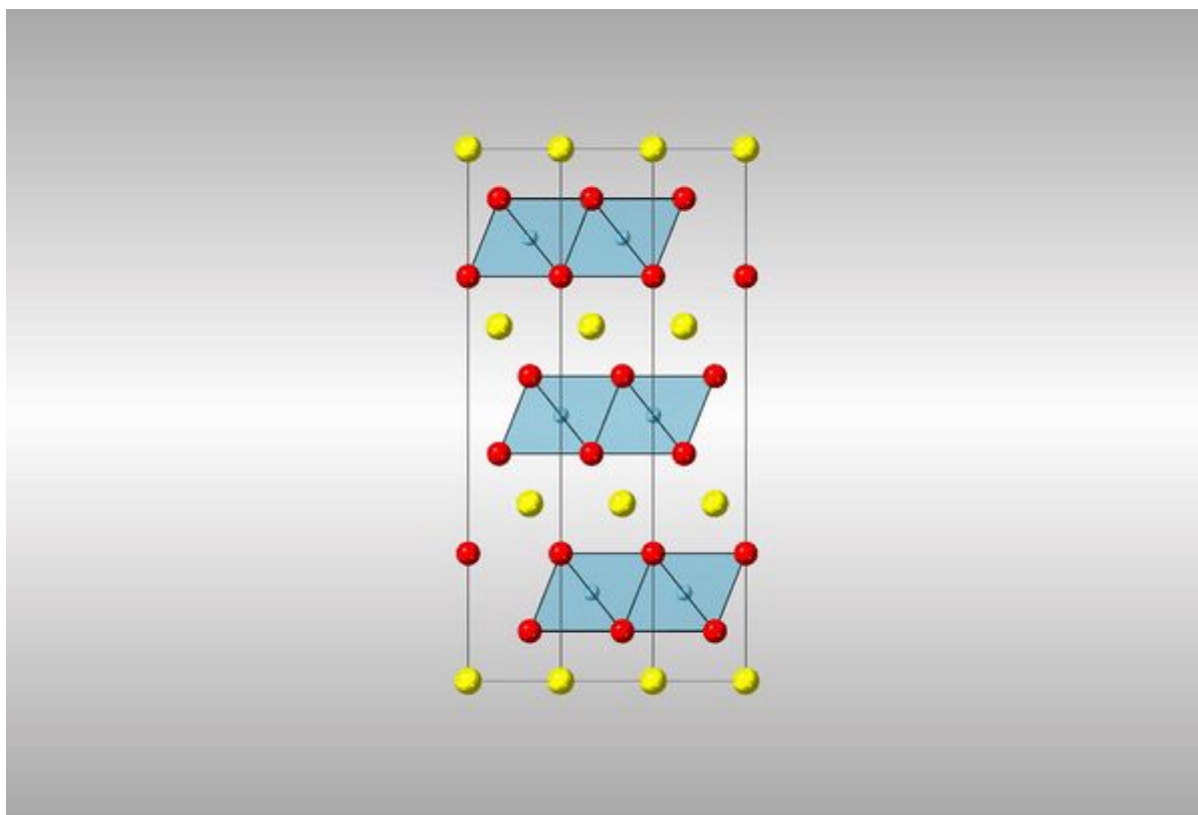
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EDITORIAL

Editorial

Mike Glazer



Hearty congratulations to John Goodenough, one of this year's recipients of the [Nobel Prize in Chemistry](#) for his contributions to the development of Li-ion batteries. At the great age of 97, this has been long, long overdue. John came to Oxford in 1976, which is where he made his original discoveries. We both arrived in Oxford at the same time and we used to joke that he, a physicist by training, found himself in a Chemistry Department, while I, a chemist by training, found myself in a Physics Department. I still recall his tendency to laugh so earth-shatteringly loudly that it echoed over great distances.

In the previous issue of the *IUCr Newsletter*, we had an [article](#) on the reference to crystallography in the movie "No Highway in the Sky", and I asked if anyone could tell us of any other movies in which crystals or crystallography had figured. I received several emails and tweets pointing to the film "The Andromeda Strain"; see [Letters to the Editor](#).

I have also discovered a reference to crystals in the 2008 movie "[Journey to the Center of the Earth](#)" directed by Eric Brevig. The film is a load of scientific tosh, as you would expect of course, but approximately 34 minutes into the film, the volcanologist Professor Trevor Anderson (played by Brendan Fraser) accompanied by a young Sean Anderson ([Josh Hutcherson](#)) and the beautiful Hannah Ásgeirsdóttir ([Anita Briem](#)) arrive deep underground at a place where they find huge rubies, emeralds, diamonds and ... feldspar! The diamonds of course are outrageously enormous. At this point our hero, the Professor, announces slowly and deliberately with a look of wonder "*Crystals are frequently formed ... and found ... in volcanic tubes*". The three characters then fall through a floor made of thin layers of muscovite. I think that this is more or less the only scene in the movie that can claim any scientific credibility! Nonetheless I can recommend it if you have nothing else to do as it is quite fun to watch.



IUCr Newsletter Editor Mike Glazer (right) in discussion with *IUCr Newsletter* author Massimo Nespolo at ECM32.

We also publish a very [interesting account](#) by a young man from Senegal about his experiences in learning about crystallography through the IUCr's [Crystallography in Africa](#) initiative. His enthusiasm just shines through this article. This is a wonderful example of the way in which the IUCr does such a lot of good things around the world, and bringing the continent of Africa into our community has to be an important and welcome development for the future. It is something that a number of crystallographers from different countries and commercial companies have been working very hard to achieve, and they deserve our support.

In this issue we have another [important article](#) from Massimo Nespolo, this time on the vexed question of the use of the term “low dimensions” in crystals. This is yet another of those areas where non-specialists tie themselves into knots, especially when trying to express ideas to do with dimensionality in crystals and the space in which the crystals exist.

Fifty years or so ago when I began research in crystallography, crystals consisted of regular arrangements of atoms and molecules. And this was the way in which we usually thought of them then. We were well aware that what we were looking at was the ‘average’ structure and that in reality the near-perfect repetition of an ideal crystal was not the whole story. Over the years it has become ever

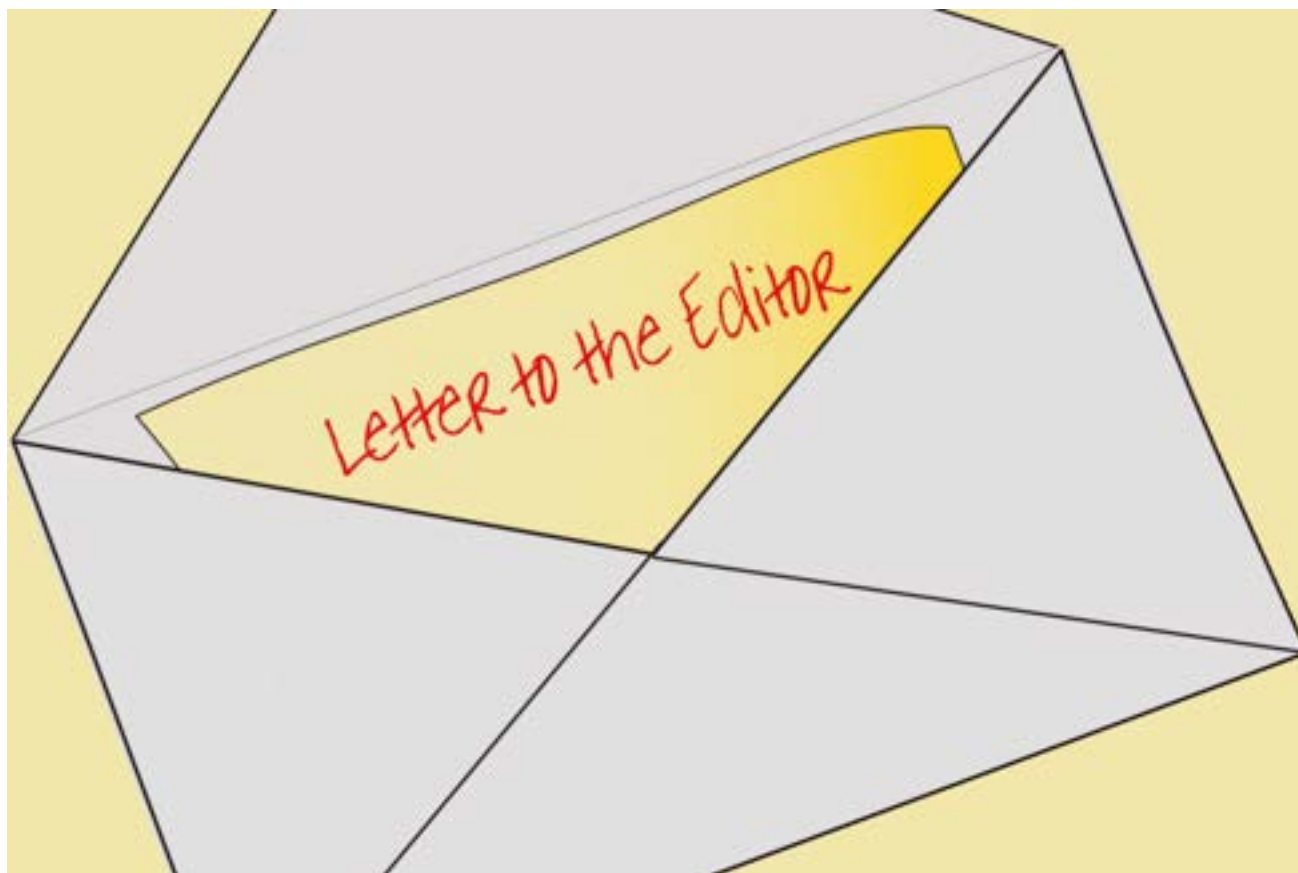
more apparent that it is in the departure from regularity where the really interesting science often resides, especially if we want to understand how physical properties arise based on the crystal structure. And so we have seen an increasing interest in studies of what we can call 'local structure'. In other words, attention is moving ever more to understanding 'real' crystals. Simon Billinge, one of the experts on real structures and the techniques used to study them, has written in this issue of the *IUCr Newsletter* an excellent [thought-provoking article](#) looking to the future of crystallography.

Finally, John Helliwell has provided a [thoughtful piece](#) on a subject that we don't often see discussed these days, but is in the tradition of the thinking of some of our great crystallographers of the past such as Lonsdale, Bernal, Hodgkin and Pauling.

If you want to comment on this, or anything else relevant to crystallography, the IUCr, etc., do please [email me](#) with your thoughts and we can then publish them in following issues either as separate articles or as Letters to the Editor.

LETTER TO THE EDITOR

Letters to the Editor



Crystallography in the movies (1)

Thank you for your article on [Crystallography in the movies](#). I was actually planning to talk at last year's ACA meeting on crystals and pop culture. I was deterred by other more pressing matters.

One good example of other mentions of crystallography in films is the 1969 Polish movie "[The Structure of Crystal](#)" directed by Krzysztof Zanussi. Actually this is not about crystals but the life of two scientists who were students together and have taken separate paths. The interesting fact is that the director actually had an advanced degree in solid-state physics so was well equipped to deal with the subject matter.

I, for better or worse, love bad movies. Of course, in the 1950s there is one with monster crystals. It is entitled "[The Monolith Monsters](#)" and made in 1957. Anyone with a knowledge of crystals will get great amusement watching this film. There is no evidence that anyone connected with it had even the most elementary knowledge of science. The idea of being threatened by immobile, huge crystals that kill by collapsing on anything beneath them is totally absurd. Later, crystals were replaced with a mobile, amorphous material that was "The Blob." Guess it is too hard to grow crystals that move.

Phillip E. Fanwick

Purdue, USA

Crystallography in the movies (2)

Reading your interesting article [Crystallography in the movies](#) and the call to report occurrences of the field, I decided to contact you.

This is about the book and the movie of Michael Crichton's *Andromeda Strain*.

If I recall well a molecular structure (or at least a look-alike) of a B_{12} -like huge ring structure is shown in both places. Quite frankly, I am not 100% percent sure of the movie.

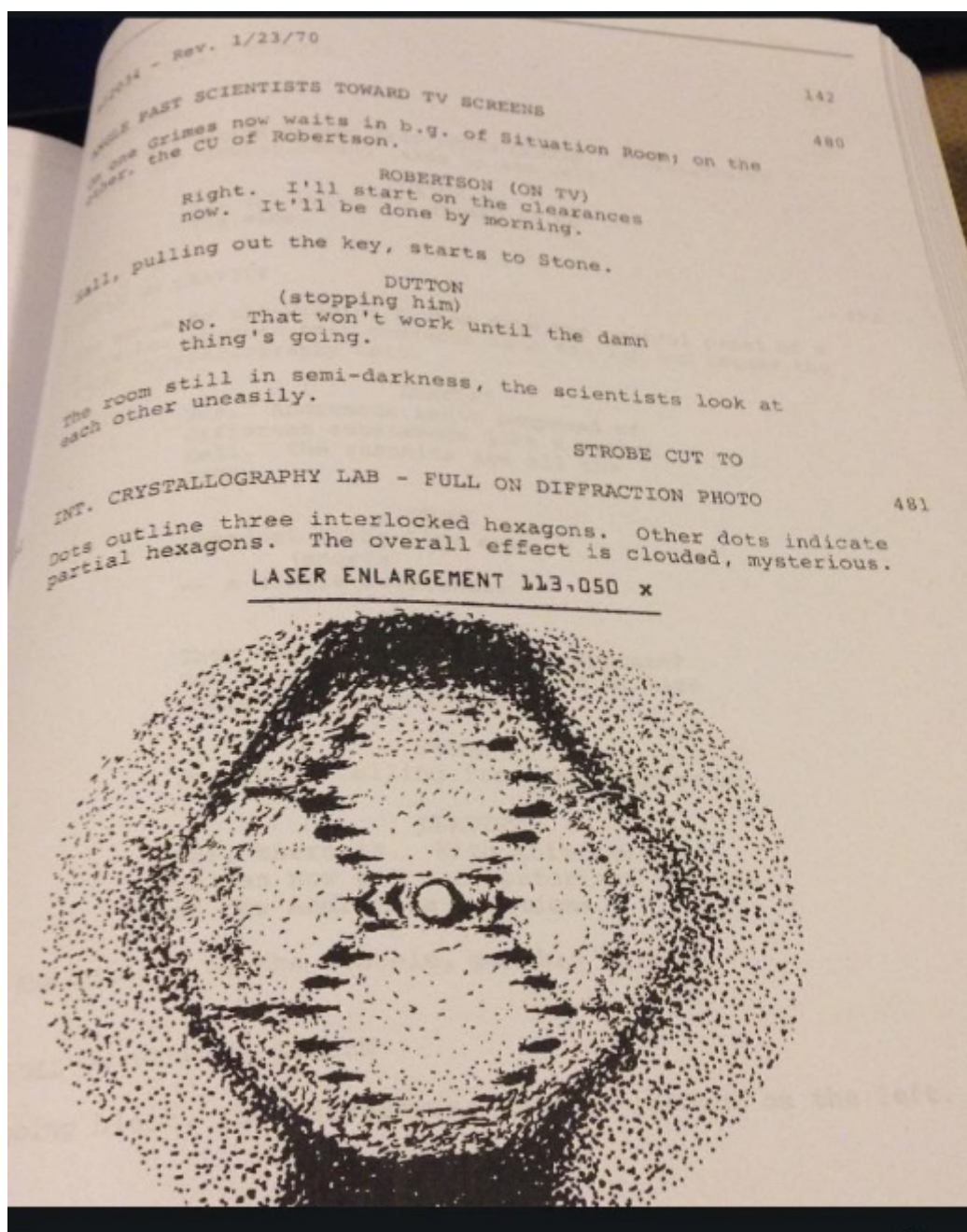
Whether X-ray crystallography is literally referenced to, this is yet another uncertainty in my memories.

Most probably this all may be known to you or to many other colleagues, too. Nevertheless, I decided to write to you in the hope of not being quite superfluous.

Mátyás Czugler

Hungarian Academy of Sciences

Editor: Several people (by Twitter) have pointed to the film *Andromeda Strain* as an example of crystallography in the movies. It can be seen [here](#). Crystallography is specifically mentioned, as shown in the following image of the script.



And for Dr Who fans ...

To add to your notes about mentions of crystals and crystallography in the movies, I feel I should add a couple of references from my favourite sci-fi TV show – *Doctor Who*. As many of your readers will know, this BBC drama has been running, on and off, since 1963, and there is therefore a wealth of material from which to draw.

Firstly, a four-part serial made in black and white in 1969, entitled “The Krotons”, concerned a race of crystalline creatures (the eponymous Krotons) who were reanimated (and grown from vats!) thanks to an inadvertent influx of mental energy from our hero, the Doctor, portrayed at the time by Patrick Troughton. Spoiler alert – the Krotons’ biology is “based on tellurium” and they are defeated by judicious application of acid. You can find the trailer for the DVD release of this serial [here](#) – perhaps wisely, the Krotons themselves are only briefly visible at moments throughout this trailer, as they are not the greatest triumph for the BBC costume department.

More notably, in 1975, in the final episode of the four-part serial “Terror of the Zygons”, there is a wonderful quotation which I used in my PhD thesis. The Zygons, a race who use “organic technology” and can change their shape to mimic human form, are hiding out in their spaceship, having been dormant for many years, but now feel ready to emerge and take over the world as a replacement for their own devastated planet, using the Loch Ness Monster (don’t ask!) as their weapon. The Doctor, by now in the form of the very well-remembered actor Tom Baker, has been captured by the Zygons but has interfered with a camera in his cell in order to send a signal about the spaceship’s location to the outside world. In the process he has been rendered unconscious by a large electric shock. The Zygons’ leader, Broton (although currently in the human form of a Scottish aristocrat – again, don’t ask!) and a colleague discover the Doctor’s prone form – at which point Broton utters the immortal line: “I underestimated his intelligence, but he underestimated the power of organic crystallography!”. I think we can all agree with that!

In contrast to the Krotons, the Zygons most certainly were an achievement for the 1970s BBC costume department – and they have reappeared several times in recent *Doctor Who* series, although sadly with no further mention of “organic crystallography”!

Steve Maginn
Cambridge, UK

Crystallography in the comics

The young illustrator Till Lukat and his colleagues from ERCcOMICS are publishing in the web a story based on my research in the ERC project Prometheus. After the release of five chapters, I am convinced that it is a simple and funny way to learn about science, discoveries, field trips, crystals, life, minerals, etc. I think it is a nice reading for children but also for almost everybody. I wonder if you can help to disseminate it among crystallographers. The comic is entitled “Something in the water” and is being published [here](#).

Juan Manuel García-Ruiz
Granada, Spain

COMMENTARY

Lab in a DAC - high-pressure crystallography as a powerful tool to study chemical interactions and chemical reactions

Elena V. Boldyreva



Figure 1. The author of this commentary with Andrzej Katrusiak in 1999 at the 18th IUCr Congress in Glasgow.

It is my great pleasure to write a scientific commentary on a recent review by Andrzej Katrusiak (Katrusiak, 2019). Time goes fast, and I have hardly noticed the two decades after the IUCr Congress in Glasgow in 1999, where I first met Andrzej in person (Fig. 1) and we could exchange our experience in high-pressure single-crystal diffraction studies of intermolecular interactions in the crystals of organic compounds. I had just entered this field in which Andrzej has been already active as one of the pioneers (Katrusiak, 1991). There were not so many people at that time who were interested in this topic.

Since that time both the hardware [diffractometers, diamond anvil cells (DACs)] and the software have developed to such an extent that a single-crystal high-pressure X-ray diffraction experiment can provide data of a completeness and precision that enables structure solution and refinement for unknown phases of great complexity, so that even an electron charge density analysis becomes possible (Casati *et al.*, 2017). Detailed studies of chemical bonds, intermolecular interactions, subtle details of structural transformations of organic crystals under extreme conditions became mainstream in chemical crystallography (Boldyreva, 2018). Research on hydrostatic compression can also be very helpful in order to understand the structural transformations at ambient pressure (Zakharov & Boldyreva, 2019). The

sample sealed in the DAC can be compressed and heated to the chosen starting pressure and temperature and then processed by changing their values. In these changing conditions one can investigate the stability regions of a compound and its phase transitions, and this information can be used for drawing the pressure-temperature (p-T) phase diagrams, in a similar way as done in high-pressure thermal analysis and calorimetry. The extreme conditions in the DAC can be applied for performing chemical reactions which otherwise would require catalysts, would proceed with much smaller yields or would not proceed at all.

The recent review by Katrusiak (2019) gives a personal overview of this exciting field. When DACs were first designed and manufactured 60 years ago, the main interest of researchers was focused on studying minerals and inorganic compounds. The progress of solving structures of organic compounds at high pressures can be illustrated by an increase in the number of crystal structures deposited in the Cambridge Structural Database (Groom *et al.*, 2016), reaching 2500 entries by the end of 2019. One relatively short article cannot cover the whole variety of high-pressure crystallographic experiments, the new designs of high-pressure equipment, computer programs for theoretical computations for high-pressure structures and for the interpretation of high-pressure data. Therefore, this research perspectives article focuses on selected aspects most relevant to crystal engineering and the research results changing the understanding of concepts in materials chemistry, undoubtedly biased by this author's personal interests. Still, the author and his research group have performed such extensive and variable research at high pressures throughout the decades that even being based mainly on a personal experience, the paper gives a balanced and multi-faceted overview of the field.

In the early years of high-pressure X-ray diffraction studies a researcher was excited to find a new high-pressure polymorph and to solve its structure. Nowadays, the challenge is to find some universal laws and rules of high-pressure transformations. The paper by Katrusiak (2019) suggests some of such possible rules. In particular, the author discusses the role of pressure-transmitting fluids in the compression of solids, the reasons why compression on cooling and on increasing pressure can be drastically different, and why the rule of inverse effects of temperature and pressure that has been formulated for inorganic solids often does not hold for organic compounds, why the inverse relation rule does not apply to the symmetry relations between low-pressure and high-pressure phases. The problem of predicting if a multi-component crystalline phase will form or, on the contrary, decompose on hydrostatic compression is discussed using solvates, hydrates, salts and co-crystals as examples. The increase in coordination numbers in the high-pressure phases as compared to the ambient-pressure counterparts is discussed and compared with an alternative possibility of increasing the crystal density by filling in the voids by guest molecules of penetrating fluids. Structural effects induced by high pressure in crystals can be so strong that they cannot be regarded solely as a physical transformation, as they change the chemical character of substances, even before the chemical reaction actually takes place. For example, the bond lengths, molecular conformation, coordination and interactions can be reversibly changed and correlated with the properties of materials under study. Thus, high pressure can induce changes in the chemical bonding similar to those characteristic for chemical reactions. This can considerably facilitate the research on functional materials in the search for their structure-properties relationships. Examples of such transformations are also given.

In general, this paper by Katrusiak represents a significant step forward in attracting attention to the new possibilities that high-pressure crystallography opens for chemical crystallography and the research of molecular materials. I would recommend it as a very informative and stimulating read to a broad community.

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COMMENTARY

A potential difference for single-particle cryo-EM

Peter B. Rosenthal

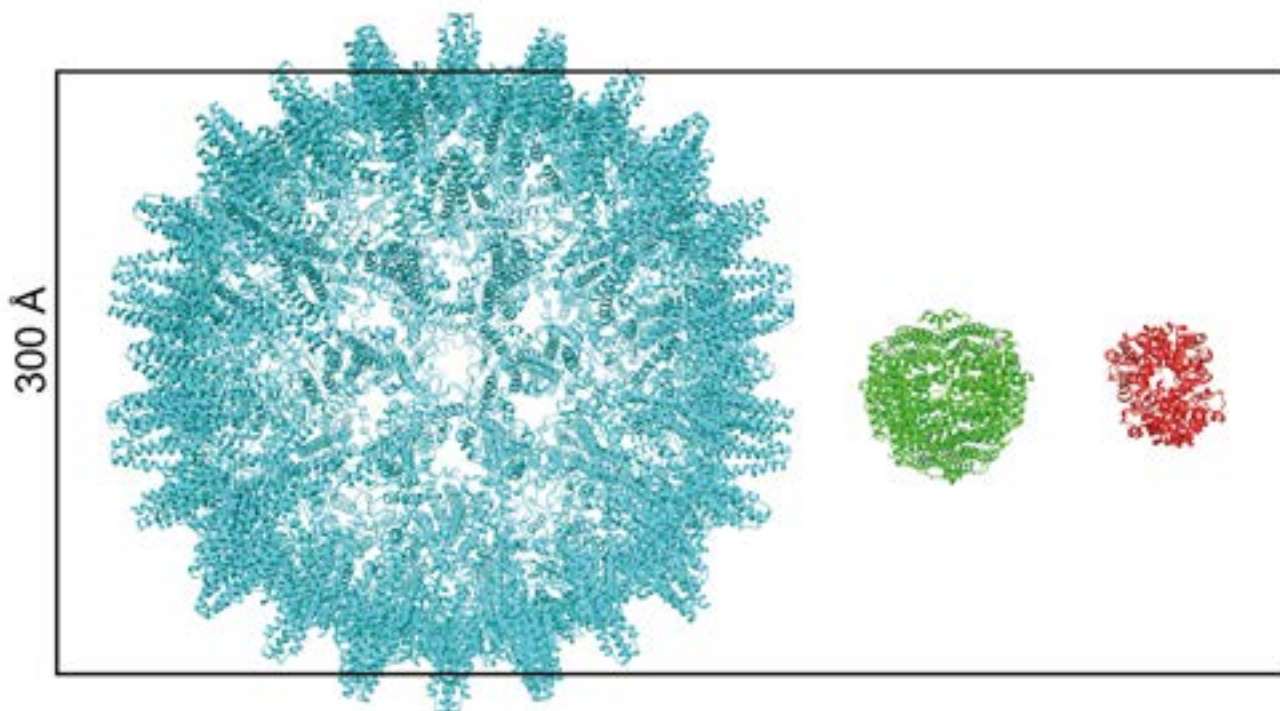


Figure 1. Three of the five single-particle specimens studied using 100 keV electrons in Naydenova *et al.* (2019) showing relative sizes: hepatitis B virus capsid (cyan), DPS (green) and haemoglobin (red). The vertical dimension of the bounding box is 300 Å.

Advances in experimental and computational methods for single-particle cryogenic electron microscopy (cryo-EM) have transformed the field of structural biology by making it possible to calculate high-resolution maps of proteins and nucleic acid assemblies without crystals. Efficient electron detectors and movie-mode data collection have been key to the resolution jumps that have been achieved for low molecular mass, asymmetric specimens. However, cryo-EM has not yet reached its theoretical limit for structure determination from small numbers of particles or from small molecular mass specimens (Henderson, 1995). Better imaging and computation together are helping to identify and hopefully find solutions to problems, such as beam-induced movement, that may further enhance this already successful technique.

Cryo-EM structure determination proceeds by recording and averaging low dose images of frozen-hydrated specimens embedded in a thin layer of vitreous ice. The structural information in images is related to the ratio of useful elastic electron scattering events to inelastic events that only cause damage and do not contribute to image contrast. A recent study (Peet *et al.*, 2019) reports new measurements of these electron-specimen interactions for 100 keV and 300 keV electrons, the energy range of electrons commonly used in biological microscopy. The study concludes that for a thin specimen

of thickness of about 300 Å, e.g. protein molecules in a somewhat larger ice layer, the optimal choice of voltage is 100 kV. For thicker specimens, including many studied in the growing field of cryotomography, higher voltage is beneficial.

This conclusion contrasts recent practice in single-particle cryo-EM, where higher electron acceleration voltages have been favoured because of their greater penetration, reduced multiple scattering and less sensitivity to electron optical aberrations and specimen charging. Indeed, most high-resolution single-particle structures come from 300 keV instruments equipped with a coherent field emission gun (FEG) source and with direct electron detectors (and often an energy filter). There have been studies emphasizing that high-resolution structures can be obtained at 200 keV (Herzik *et al.*, 2017, 2019). Furthermore, the efficient direct electron detectors in current use in cryo-EM have been optimized for 300 keV and perform well at 200 keV. At lower energies, backscattering of electrons leads to degradation of signal.

In the article by Naydenova *et al.* in this issue of **IUCrJ** (Naydenova *et al.*, 2019), the same research team has followed their earlier analysis with a practical demonstration that structure determination of challenging biological specimens can be performed using 100 keV electrons. Their experiments combine all the necessary instrument features and show that many of the problems associated with low voltage can be addressed. The study was performed on a 200 keV microscope with a coherent FEG electron source, though operated at 100 keV. Commercial instruments with lower voltage (a maximum 100 or 120 kV) are not equipped with FEG sources. A key feature of the new study is the use of a hybrid-pixel detector (Faruqi & McMullan, 2018), developed for X-ray diffraction studies, the Dectris EIGER (Dinapoli *et al.*, 2011). Imaging and reconstruction are applied to five single-particle specimens of varying sizes and masses: hepatitis B virus capsid, bacterial 70S ribosome, DPS (DNA protection during starvation protein), catalase and haemoglobin (see Fig. 1). Notably, the DPS protein (220 kDa) was resolved to 3.4 Å.

Additional concerns have caused pessimism about high-resolution work at low voltage. There is a greater effect of beam tilt on image phases at lower voltage. However, beam tilt, as well as other aberrations, is modelled successfully by the software used for reconstruction in this study, *RELION-3* (Zivanov *et al.*, 2018). Another potential problem at low voltage is that the depth of field (or equivalently, the greater curvature of the Ewald sphere) becomes important for thick specimens at high resolution, and the images are no longer true projections of the structure. Though not a concern at the resolutions reported in the present study, computational correction has been demonstrated (Russo & Henderson, 2018; Wolf *et al.*, 2006). The effect of chromatic aberration is worse at lower voltage and ultimately limits resolution.

This is just the beginning for high-resolution work at 100 keV: though the performance of the detector was excellent, its area was small (1030 × 514 pixels), so an inefficient way of obtaining the large number of particles ideally required for high-resolution work. Nor did the detector count individual electrons. The new results reported here should fuel research on the detectors optimized for lower voltage and microscope platforms that possess features proven to be important in their higher voltage relatives.

The authors describe requirements for a future 'ultimate' single-particle microscope operating at 100 kV for structure determination to better than 2 Å. With coherent illumination and a large pixel format electron counting detector, the authors specify several ways in which the required small chromatic aberration may be achieved. But perhaps of greater immediate impact, the authors propose a microscope optimized for single-particle data collection to 3 Å or somewhat better, still capable of obtaining near-atomic maps and models, but also suitable for specimen screening. In many investigations, as in the one reported here, sample preparation is not uniformly ideal. Until sample preparation problems are solved more generally, optimization requires significant time on a lower-end screening instrument, but can ensure subsequent success on a higher-end instrument. To be predictive for success at high resolution, the standard for a screening instrument is still quite high. More than showing the shape of particles in ice, it ideally allows one to detect high-resolution features (secondary

structure) in 2D image averages, an early step in image analysis, and identify a wide range of orientations, a requirement for isotropic resolution. Voltage is a surrogate for size and cost, both for the instrument and environment to house it. The authors envision that such affordable instruments (and available software) will make cryo-EM more widely accessible. This will reduce some of the (high) tension associated with the rapid growth of the field.

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FEATURE ARTICLE

Crystallographic flatland

Massimo Nespolo



The discovery of quasicrystals represented such a paradigmatic shift in the way we look at condensed matter that even the definition of a crystal had to be amended to take into account materials that violate the three-dimensional (3D) periodicity, which had been for so many years considered the most fundamental feature of a crystal. Currently, the [official definition](#) reads as follows: “A material is a crystal if it has essentially a sharp diffraction pattern”, but this has been the subject of a number of discussions (e.g. Lifshitz, 2007). In particular, the definition in reciprocal space does not fit everybody’s taste as the physical object has its physical existence in direct space. A higher-dimensional approach seems more satisfactory because it “elegantly restores hidden symmetry and correlations of quasiperiodic structures” (Steurer & Deloudi, 2009) and encompasses other aperiodic structures (incommensurately modulated structures and co-crystals) as well; although some aperiodic structures can be described as periodic without the need for a higher-dimensional space, but by changing the geometry of the space (Kocian, 2013). Crystallographers are today used to working with higher-dimensional spaces, even up to six dimensions.

In recent years lower-dimensional spaces, instead of higher-dimensional ones, have increasingly attracted attention, in particular from material scientists and crystal engineers. Journals, even serious ones, are flooded with publications about “low-dimensional materials” endowed with extraordinary properties. Non-specialists are tempted to believe that after superspaces it is now the turn of subspaces to reserve surprises to those daring to explore them. Unfortunately, it all comes down to a fundamental misunderstanding by authors who seem to ignore the notion of *subperiodicity*. Not only is there nothing conceptually new in these materials, so that one could say “much ado about nothing”, but the

misunderstanding may prevent the investigators from using the mathematical tools suitable for their materials, which were well known long ago. I briefly addressed this problem in the *Journal of Applied Crystallography* (Nespolo, 2019); here I try to explain it to a less-specialised public.

Can a material exist in a low-dimensional space?

The extravagant expression “low-dimensional material” is showing up even in high-impact journals. For example, Voiry *et al.* (2018) wrote about “low-dimensional catalysts” and in their [Figure 1](#) they describe “0D nanoparticles, 1D nanowires/nanotubes and 2D nanosheets”. A quick look at the figure shows beyond any doubt, and without any surprise, that these materials possess a volume and as such are perfectly 3D objects. The trap in which the investigators fall – and this is really surprising! – is in mistaking the number of dimensions of that space within which the material shows periodicity for the number of dimensions of the space in which the material occurs. The so-called “0D nanoparticles” are finite (non-periodic) 3D particles. The so-called “1D nanowires/nanotubes” are 3D nanomaterials that are periodic along one direction and non-periodic along the two other directions of the space. The so-called “2D nanosheets” are 3D sheets that are periodic along two directions and non-periodic along the other direction of the space. Quite obviously, there cannot be any 0D, 1D or 2D material ($D = \text{dimensional}$)¹; these materials are built by 0P, 1P or 2P ($P = \text{periodic}$) building blocks (*modules*: bricks, rods, sheets) and are simply modular structures (Ferraris *et al.*, 2008), which have been the subject of investigation for almost a century (Umayahara & Nespolo, 2019).

The confusion is far from being devoid of consequences. The physical, chemical and mechanical properties that make these materials technologically interesting depend on how each of the modules is arranged with respect to the others. One of the challenges in crystal engineering is to optimise this arrangement so as to maximise the properties of interest while at the same time obtaining a stable material. Now, depending on the structure of both the bulk and the surface of the modules, the arrangement can usually be realised in a finite (often small) number of variants, which can be represented by a mathematical operation that maps the modules, and these operations depend on the symmetry of the module. If the module was 0D, 1D or 2D, it could be embedded into (exist in) a 0D, 1D or 2D space, and its symmetry group would be the point group containing only the identity (how do you move in a 0D space?), a line group (1D space group) or a wallpaper group (a 2D group), respectively. The modules are actually embedded (existing) in the ordinary 3D space but are periodic along a subset of dimensions. Their symmetry groups are 3D but *subperiodic*: point groups for 0P modules, rod groups for 1P modules and layer groups for 2P modules (see table below).

If the module was	its symmetry group would be	but because it is	its symmetry group is
0D	{1}	0P	point (non-periodic) group
1D	line group	1P	rod (monoperiodic) group
2D	wallpaper group	2P	layer (diperiodic) group

Subperiodic groups have been well known for almost a century (Niggli, 1924; Polya, 1924; Speiser, 1927; Alexander & Herrmann, 1929; Hermann, 1929) and are described in detail in Volume E of *International Tables for Crystallography* (Kopský & Litvin, 2010). There cannot be an excuse for mistaking a subperiodic group for a low-dimensional group.

The possible arrangement of successive modules that corresponds to a coherent interface allowing the establishment of chemical bonds between a pair of modules corresponds again to a subperiodic group. This group is obtained as the intersection of the subperiodic group of the two modules in their respective orientation and position. Failing to recognise the subperiodic nature of the module prevents symmetry

analysis, which is key to predicting the possible juxtapositions of modules compatible with their structure and surface.

Getting a general picture

Such an awkward description of materials reminds me of E. A. Abbott's satirical novella *Flatland: A Romance of Many Dimensions*, in which the main character, A. Square, describes the 2D world in which he lives. Being born and grown in a 2D world, for him the Universe can only have two dimensions. On the eve of the third Millennium he dreams of visiting a 1D (Lineland) world, inhabited by points who can see him only as a set of points on a line. This dream represents the beginning of an adventure that eventually profoundly shakes the foundations of his (flat) conscience. He receives a visit from an inhabitant of a 3D world (Spaceland), a Sphere, which he is unable to see as anything other than a circle. The idea of the existence of a third dimension, subversive in a 2D world where your position in the society depends on the number of edges you have, infiltrates his soul and opens his mind to new dimensions, to the point that he tries, without success, to convince the Sphere of the theoretical possibility of the existence of fourth and higher spatial dimensions. Later, the Sphere comes to him again in a dream to introduce him to Pointland, a 0D world where a point, the sole inhabitant, perceives any communication as a thought originating in his own mind.

Crystals in Spaceland are 3D objects. Some of them are modular structures built by subperiodic, but not low-dimensional, modules. If we turned our eyes over the 2D crystallographers of Flatland, we would look at them with compassion, for they are unable to grasp the 3D nature of the crystals of which they can experience only a section. They indeed describe our crystals as 2D objects whose symmetry is a wallpaper group, but only because they cannot realise the 3D nature of the object: we do, and it is simply meaningless to adopt the viewpoint of Flatlanders. We can go further, and turn our eyes over the 1D crystallographers of Lineland, for whom our crystals are just a 1D object whose symmetry is a line group: in this case we would share with Flatlanders the compassion for these dimensionally limited colleagues. It is hard to imagine how a crystallographer of Pointland would experience our crystals.

We crystallographers of Spaceland are today acquainted with the idea of materials existing in higher-dimensional spaces that we experience as a projection in our world. How would crystallographers of Superspaceland look at us? What we describe as aperiodic crystals would be considered ordinary crystals of Superspaceland. Among these, there would certainly be modular structures with interesting properties built by subperiodic modules, which show periodicity along only three of the four (or more) dimensions of Superspaceland. Superspaceland crystallographers would most likely look at us with the same sorrow we feel for Flatland crystallographers because of our incapacity to grasp the 4D nature of the crystal.

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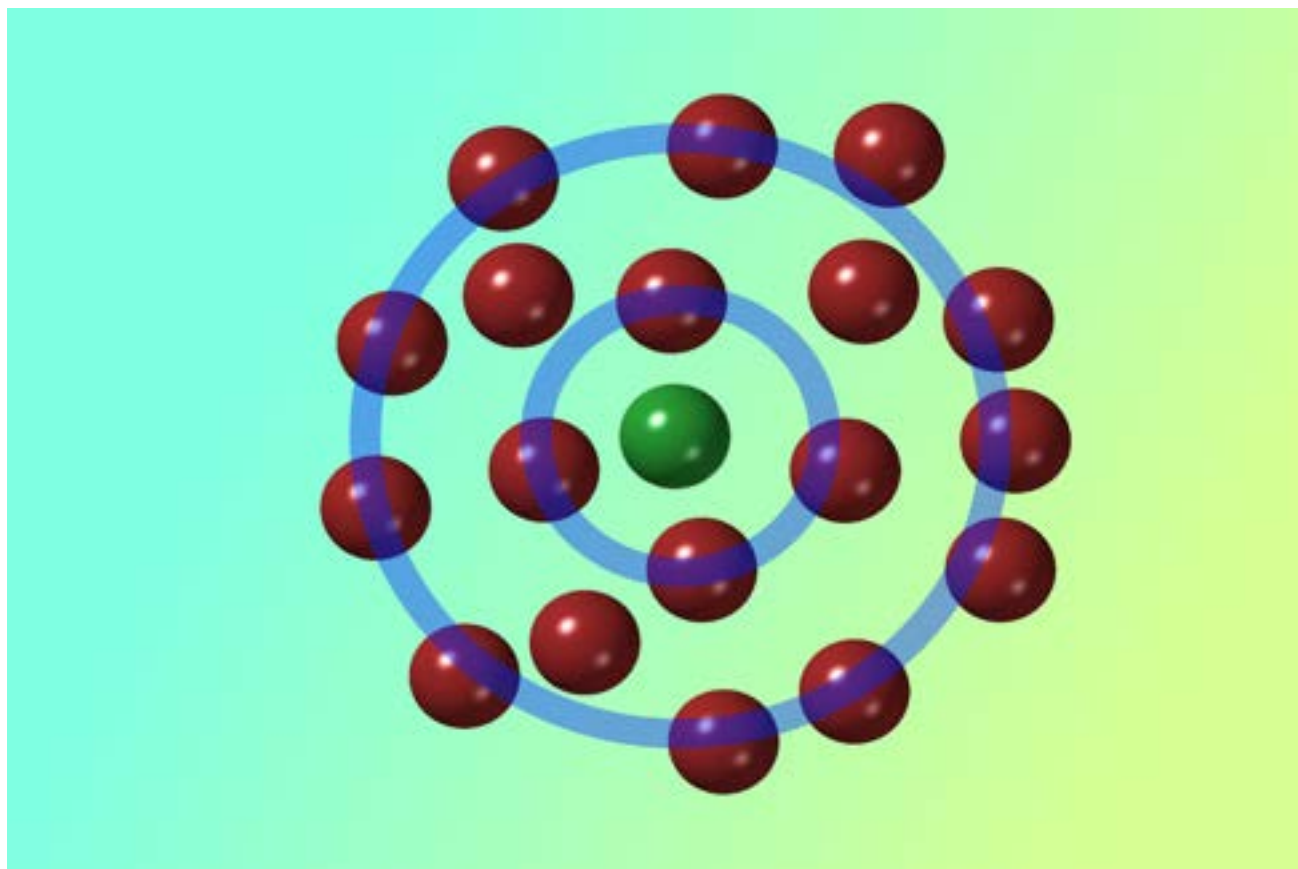
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1 Even graphene does not have zero thickness!

FEATURE ARTICLE

21st century challenges: structure beyond crystals

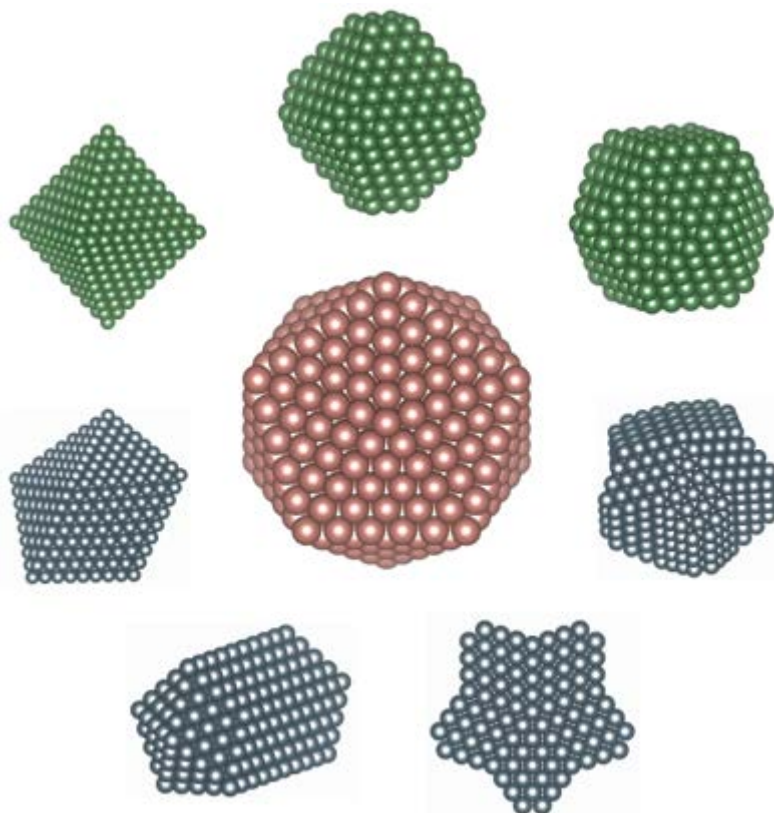
Simon J. L. Billinge



Largely speaking, crystallography is a solved problem. Wait, what? How can I write that as the opening sentence in an article in the newsletter of the august IUCr and not upset the entire readership of crystallographers – my colleagues? But it is a statement that we should face full on, both to celebrate and to examine for our own survival as a community of researchers. When crystallography was born at the end of the first decade of the 20th century, the very existence and nature of atoms were in question. Boltzmann died in 1906 in conflict with the powerful German positivist school of Ernst Mach without ever having full validation of his statistical mechanics through the validation of the discovery of atoms.¹ The nature of X-rays was still being sorted out (Barkla, 1909) and Rutherford's experiment to establish that the atom had all its mass in a tiny point at the center would not be published until 1911 (Rutherford, 1911). Indeed, arguably, it was the X-ray crystallography of Max von Laue, Paul Knipping and Walter Friedrich (Friedrich *et al.*, 1913; reproduced from Friedrich *et al.*, 1912) and the Braggs (Bragg, 1913; Bragg & Bragg, 1913), taking place in the period right before the First World War, which settled both questions: X-rays are short-wavelength electromagnetic radiation waves and, without doubt, stuff is made of Rutherford-esque atoms in regular arrangements. Over the proceeding 100 years or so, the brilliance of our radiation sources increased by many orders of magnitude; the simplifying power of applied mathematical concepts such as space-group theory (Aroyo, 2016) applied to solving atomic arrangements in crystals, and constraints coming from atomicity and the positivity of density and so on

(Giacovazzo *et al.*, 1992), made the inversion problem – given this X-ray pattern to what was the 3D arrangement of atoms – tractable.

In this period, the power of computing exploded, so that by the end of the century we were routinely solving the structures of rather large, complicated and low-symmetry proteins (Karthikeyan *et al.*, 1999), and even larger objects like viruses (Harrison *et al.*, 1978). Structures of straightforward inorganic and small-molecule crystals can be solved automatically, at the push of a button, on a modern laboratory diffractometer, and the biggest problem in protein crystallography is now often getting the crystals to grow rather than doing the crystallography on the resulting data. Generically speaking, this is very much the description of a solved problem: if you can make a machine that gives the answer at the push of a button, the problem is solved. So maybe it is time to pat ourselves on the back, kick up our feet and wind up the IUCr, satisfied in the warm glow of a “a good job well done”.

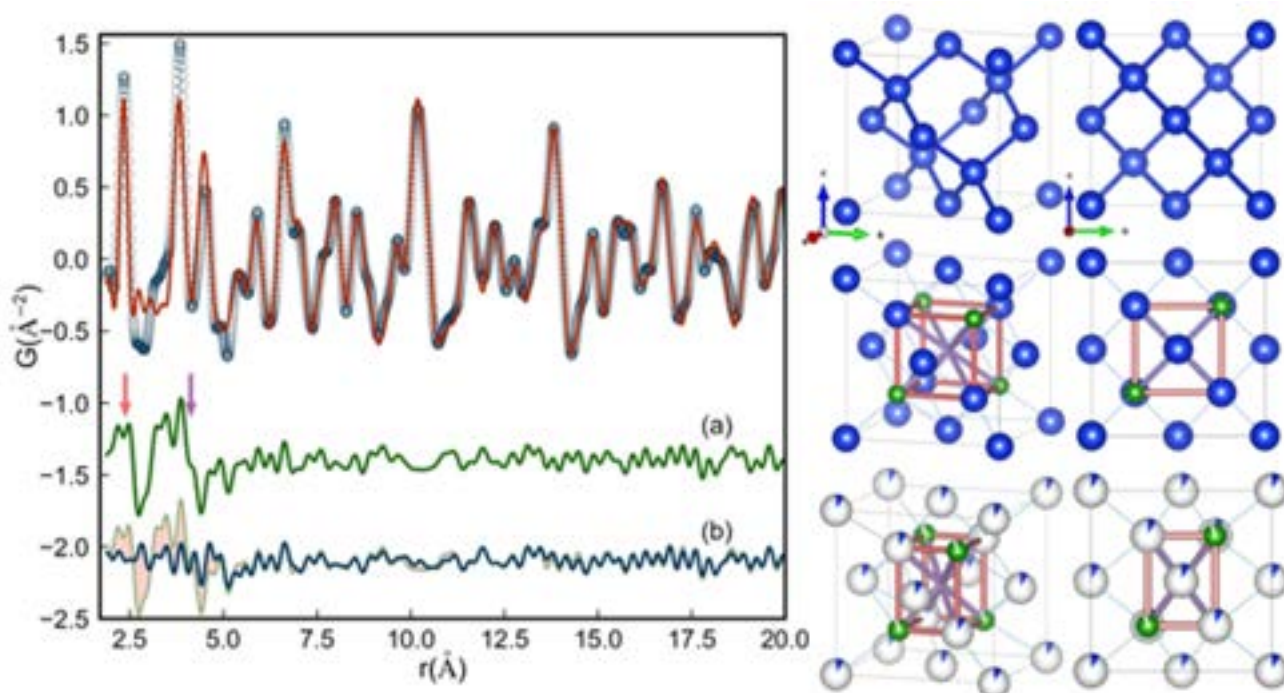


Metallic nanoparticles form structures that are not space filling and cannot form in bulk materials. Here we show metallic nanoparticle cluster models, which may be tested against PDF diffraction data, that illustrate a number of different families, including truncated f.c.c. structures (green), different decahedral motifs with pentagonal arrangements of tetrahedrally shaped f.c.c. subdomains (blue) and icosahedral structures (red). See Banerjee *et al.* (2018) for more details. Image credit: Soham Banerjee.

However, I beg to differ. Apart from the rather large number of crystal structures that can't yet be solved at the push of a button, and the large number of future crystallographers that we need to train, we are actually facing a much more fundamental problem in structure science. Rather than kicking up our feet, we need to be rolling up our sleeves. I believe that our community, and its particular knowledge and skill set, will be as much at the forefront of solving humankind's problems in the 21st century as they were in the 20th. The IUCr can, and should, be providing leadership to the much broader scientific community moving forward, well beyond the large shadow of its past successes. Furthermore, it will not be the IUCr in isolation but in partnership with the materials, chemistry, physics, geology and biological communities, and it will benefit us to be outward looking, as is our tradition.

Let's explore this further by thinking about some of the biggest challenges facing humankind and our potential role in finding technological solutions to them. Climate change is a central concern. At the heart

of stabilizing the situation is to move to fully renewable energy sources on the one hand, and possibly sequestering carbon on the other. These are materials science problems. Why do I say that? Most of the Earth's energy comes from the sun, so a major aspect of sustainable energy means harvesting that energy from the sun sustainably. We know how to do this, so arguably this is already a solved problem. For example, we can turn sunlight into electricity directly by using photovoltaics. But how do we do this at scale? We need photovoltaics that are inexpensive to manufacture and that can cover vast areas of the surface of the earth without destroying our environment or killing habitats. They also need to be made of earth-abundant and environmentally friendly materials. They only work during the day, so we need to store the energy for the night time. We know how to do that, we use batteries! But we need to take these to scale, giving temporary storage to terajoules of energy. A large city uses of the order of 10 GW^2 of electricity, so ten thousand million joules of energy per second. Far from the equator, in the winter, the days are short and the nights are long, so vast quantities of electrical power must be stored for this to work. It is another materials problem. We can store energy as liquid fuels. Nature did this. Sunlight was converted to electrical energy by photosynthesis and stored as chemical energy, principally in C—C bonds. The plants that were not recycled by bacteria settled in anaerobic environments turning into oil, gas and coal, fossil fuels for us to plunder later. We can replay this playbook by developing artificial processes for using the sunlight to run reactions backwards (for example, turning water into hydrogen and oxygen), but they have to be more efficient than plants because we need to be converting the energy at the same rate we are using it, not collecting it for two million years and then using it over two hundred years. This is also a materials problem: finding robust, inexpensive, earth abundant (*etc.*) materials for catalysing these uphill reactions. Then there is the fresh-water challenge. We know how to purify water, but what materials, in what devices, can do this at scale with manageable energy inputs and without pollution? Food. We had a green revolution that banished starvation from a technological point of view (there are excesses of food in the world right now so the presence of starvation is presumably a political and sociological issue rather than technological). But the revolution involved processes, such as the production of active nitrogen and phosphorous, that are not sustainable from an energy perspective, a CO_2 emissions perspective and a raw-resource perspective, not to mention pollution of the environment with salt, nitrates and phosphates. The world population is cruising through seven billion on its way to ten billion before it will stabilize and come back down. We need another green revolution that is sustainable, but also at scale and non-polluting, to feed this new world population. Another materials problem. Disease. Again, we have cures for many, though far from all, things, but how do we bring this to scale, so that the cures are cheap and abundant?

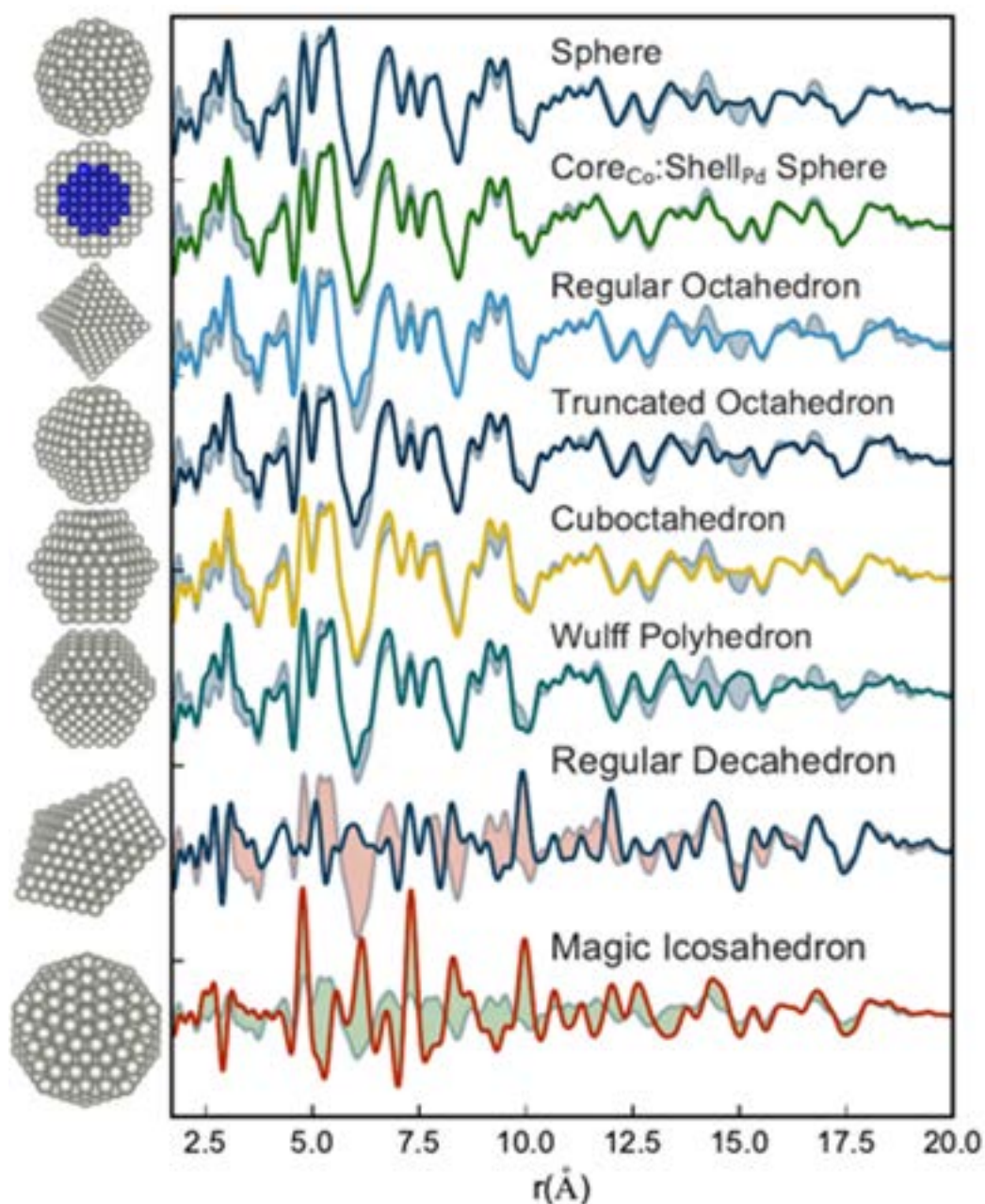


Using very non-equilibrium laser-based methods it is possible to hyper dope boron into silicon, the world's most important semiconducting material, at doping levels that far exceed normal solubility limits and result in a material that demonstrates a tunable localized surface plasmon resonance, a property of a metal. Quantitative local structural methods based on PDF analysis of X-ray powder diffraction shown here indicate that the doped boron forms defect clusters with sphalerite- and fluorite-like nanostructures. See Rohani *et al.* (2019) for more details. Image credit: Soham Banerjee.

What is the role of crystallography, and the challenges, in this picture? It has always been the understanding of the structure–property relationship, through the intermediary of quantum mechanical models such as density functional theory (Kohn & Sham, 1965), or even just geometric insights from details of protein folds, that have led to understanding of how materials do what they do. To solve the technological problems outlined above, we need better devices built on better materials. And we need them quickly, by carrying out more targeted, less trial-and-error, materials discovery campaigns. “Structure–property relationship” contains the word structure and, no worries, we have solved the crystallography problem, right? But virtually none of the technological solutions I have hinted at above make use of perfect crystals. They use what I would call “real materials”. These are materials with defects and interfaces and heterogeneities. They can be multi-phase and nanostructured, making key use of their morphology, which is increasingly nanoscale. Many of the processes of interest, such as catalysis, take place at the surface of a supported nanoparticle, the structure of which could be very different from the crystallographic form of that same material, but even more challenging, different from the structure of the core of the same nanoparticle. The properties of materials depend sensitively on bond-length variations of the order of a few picometres to a few tens of picometres. Doped lanthanum manganite changes from an insulator to a metal when its Mn–O bond length changes by just 10 pm (Billinge *et al.*, 1996), and just a single surface trap state, a structural defect, in a quantum dot nanoparticle, can have a large effect on its optical properties and quantum yield. This kind of structural precision is commonplace in crystallography, when we are studying the “crystal structure” of a material. Even though we are typically using X-rays with a wavelength of angstroms (100 pm), we can measure bond lengths with a precision at the picometre scale. Normally, a ruler that is graded in mm steps gives a measurement precision that is on the mm scale, not 100× better than that. How is it possible that we can pull off this trick in crystallography? It is because of the periodicity of the structure, and we are interested in the average bond length. Roughly speaking, we measure the distance between atoms 100 unit cells apart with angstrom precision, then divide by 100. This trick goes out of the window when we are considering discrete particles that are either physically only a few nanometres in size or have a structural coherence that is only nanometre-sized. We need new tricks to get this kind of precision and robustness when studying aperiodic structures: structures that don't repeat periodically over long distances. The “crystallography” that we need in order to solve humankind's 21st century problems is the crystallography of “real materials” or crystallography beyond crystals. This is not a solved problem, in the sense that there is no machine where you can load the sample, press a button, and the machine tells you the answer.

Nonetheless, there is much to be optimistic about in this regard. When we have powders of nanomaterials, there are powerful total scattering and atomic pair distribution function (PDF) methods that reveal one-dimensional (1D) orientationally averaged signals of the “local” arrangement of atoms. It is still a challenge to invert such a dataset to get precise atomic information *ab initio*, but the sensitivity of these methods is now high to the point where thin nanocrystalline films of a hundred nanometres thickness can be studied quantitatively (Jensen *et al.*, 2015), where the local structure of organic nanoparticles in water at the 0.25 wt% level can be studied (Terban *et al.*, 2015), and where information about the packing of solvent ions around solute species can be explored (Zobel *et al.*, 2015). In good old-fashioned crystals we are also increasingly finding, when probed with these local techniques, that local and nanometre-scale structures exist that are different than the local atomic arrangement implied by the average crystal structure (Billinge *et al.*, 1994; Bozin *et al.*, 2019; Koch *et al.*, 2019). In other words, in these systems, the crystal structure that we can solve so readily using traditional crystallography only represents a periodic average of real local structures that are different, and lower symmetry. The average structure is recovered by averaging over different orientations of the lower symmetry

distortions. When we have a situation like this and it is possible to grow a single crystal, thanks to advances in detectors and computing, it is now possible to obtain a 3D PDF function (Simonov, 2014) that is richer in information than the 1D PDF from the powder. PDF methods are being extended to electron diffraction (Abeykoon *et al.*, 2012) to augment the ever powerful imaging modalities of individual nanograins with more quantitative, though sample-averaged, 3D structural information. Solving the structures of individual nanoobjects is also at our door. The success of cryo-EM methods for solving protein, virus and chromosome structures is now well documented (Lyumkis, 2019) and a challenge to the pre-eminence of protein crystallography for protein-structure solution. However, it is only a challenge to us as crystallographers if we define crystallography in its most narrow sense of solving the structure of crystals. If we are in the business of solving the structure of real materials, and going beyond crystals, then proponents of cryo-EM are legitimate members of our new big-tent crystallography community, which is really a community on the quest of solving atomic-scale structure whatever its form, crystalline or not. Methods closely related to cryo-EM are now being applied to inorganic nanoparticles with some success (Miao *et al.*, 2016), and so a future where we can reconstruct the atomic positions of individual atoms in a finite object are close at hand, if not yet routine. New developments in hard X-ray free-electron lasers are now opening up the possibility of studying nanostructures in a time-resolved way on picosecond time scales (Gaffney & Chapman, 2007). What happens to the photoactive material in the photovoltaic cell when light hits it? How does it respond and change its atomic arrangements? Early time-resolved experiments have been hard to interpret but the methods are getting better and technological challenges are being overcome, so these experiments are on the verge of being more robust and quantitative. Other *in situ* experiments where materials have different gases flowed over them and where the nanostructure is watched as a function of time after a perturbation are revealing that real materials are not just static like fossils but more closely resemble the living creatures before they were turned to stone (Gallagher *et al.*, 2014). Mapping real materials as a function of position, at the micrometre scale and finer, is also possible by combining tomographic methods with nanostructure diffraction probes (Jacques *et al.*, 2013). Then we can combine these modalities to study reactions as a function of time and position (Vamvakeros *et al.*, 2018). We are on the verge, as crystallographers, of being able to watch these changes in local structure as they happen and this is the route to understanding real structure-property relationships of real materials.



A recent approach using high-throughput screening of large numbers of different nanoparticle structure candidates allows researchers to understand how each model improves the difference curves (goodness-of-fit curves) of the models against measured X-ray synchrotron data, yielding new insights into the structures of small nanoparticles. See Banerjee *et al.* (2019) for more details. Image credit: Soham Banerjee.

The future of crystallography is bright, if we embrace all the diversity of material structures in all their richness and variability, and bring to bear the full range of methods we need to tease out these arrangements in all their beauty and elegance. As in the 20th century, this will fully leverage advances in sources and instrumentation, applied mathematical developments including those coming from the artificial-intelligence and machine-learning communities, and computation, and will be a key part of materials breakthroughs that are so badly needed to mitigate our global challenges. It's a great time to be a "crystallographer".

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1 A quote attributed to Mach is “Atoms? Have you seen one yet?”

2 This is estimated based on an efficient 1 GW power station being able to supply roughly 700 000 homes, and there being 7 000 000 households in New York city, a canonical large city and currently my hometown.

OPINION

What we can do towards world peace

John R. Helliwell



I became deeply interested in peace in the world as a DPhil student learning enzyme crystallography at Oxford University, UK, between 1974 and 1978 with Margaret Adams. We were based in an overall group headed by Dorothy Hodgkin and her people, Guy and Eleanor Dodson and research visitors. I learnt that Dorothy was to become President of Pugwash (1976–1988), an organisation whose main objective was "the elimination of all weapons of mass destruction and of war as a social institution to settle international disputes". Dorothy was also IUCr President in this period (1981 to 1984). Coming from a regular upbringing, *i.e.* where my father and grandfather had fought in both World Wars, I had a simple view that defence, not aggression, is what is necessary. Pugwash deepened but did not resolve my thinking away from this view. Later, by chance, I came across Kathleen Lonsdale's short book *Is Peace Possible?* My thinking was swept forward by her book and its careful analysis, summed up in the Christian saying "turn the other cheek". But, how so difficult when I thought of the scale of offensive provocations, or threats of, that we witness. Then I discovered Linus Pauling's book *No More War*, which focused on nuclear weapons. The peace that has followed their first use in 1945 is surmised to be due to knowledge that it would be a nuclear war of such magnitude that it really could not be allowed to happen.

In this somewhat random walk in deepening my thinking about these matters another step unexpectedly came in the *Times Higher Education Supplement* (THES) of 14 November 2019, where I saw a review of the book [World Peace \(And How We Can Achieve It\)](#) by Alex J. Bellamy. I bought an ecopy of the book,

which I have read carefully. It tackles the same issues afresh. That nuclear weapons are the mainstay of the modern peace since 1945 is aired in Bellamy's book on page 94.

Should we crystallographers take an interest in all this? More to the point, what can we do towards peaceful ends? It isn't in our science *but* it is in our history because of Lonsdale, Hodgkin and Pauling. So I think we should take a direct interest. I have written about this before. Several years ago when I saw that the ACA's Transactions Symposium in 2015 was on *Crystallography and Sustainability*, I submitted an abstract. In my [subsequent article](#) (pages 8 to 19), I blended our historical crystallography leaders' activities, which I mention above, with aspects of my most recent research on green (structural) chemistry applications, namely working towards better clinical outcomes with fewer chemicals. In my research for the talk at ACA2015, I was struck by the absence of striving for peace as one of the United Nations eight, at the time, sustainability development goals (SDGs), a fact that I found bewildering.

So I looked to this new book by A. J. Bellamy to further learn about these issues and what one as an individual can do to try to help. Bellamy has extensive experience and is very accomplished in the field of peace studies. There are several points to be highlighted, although the whole book is a very interesting treatment of the topic. It also provides a very long historical look back, such as at the peaceful Minoan culture (see my picture below) and scrutinises cave paintings as evidence of peace or war-like activities of our ancestors, and much more besides. Suffice to say he finally suggests improvements in our modern procedures for peace upheld as best it can by the United Nations.



More specific to us as crystallographers, I immediately checked if Bellamy's book cited Kathleen Lonsdale's book or Linus Pauling's book? But it does not. I also wondered if scientists' roles are 'only' the shortening of wars, e.g. by the [sound-ranging initiatives of W. L. Bragg in the first World War](#). But there was no mention of W. L. Bragg either; maybe that is a too-specific contribution for me to expect. But Bellamy's book has introduced me to J. D. Bernal's 1958 book *World Without War*, although Bellamy gives Bernal the briefest of mentions. At page 17, Bernal is uncompromising in his analysis of the nuclear deterrent, asking that if "each [side] could destroy the other and that between them they could destroy the rest of the world, why not accept the nuclear stalemate and dismantle the whole apparatus[?]"

Bernal's book goes on to describe his vision that "Only in a world without war would there be ... the possibility ... to satisfy human needs." Indeed it is still true today; the [expenditure on violence per year is USD14.8 trillion, i.e. 12.4% of the world's GDP](#). Imagine what humankind could do if it would agree to peaceful objectives.

Anyway, the historical context of 50 to 100 years ago is one thing but what about now? The current era is best described in Bellamy's Chapter 8 entitled "Towards World Peace". The UN Charter is described and to a degree is dissected. There is clearly a specific problem of the power of a veto or "threatened vetos" of the members of the UN Security Council. This does seem a "fundamental flaw in the international security architecture" (page 185). I also agree that the "challenge isn't to reinvent the institutional architecture but to make it work better". On the last page of Bellamy's book (page 213) is a call to "everyone to assume some responsibility towards world peace". The final quotation goes to the UN Secretary General Ban-Ki moon in 2016:

"Peace is not an accident. Peace is not a gift. Peace is something we must all work for, every day in every country".

CERN in Geneva was established not only to find out new fundamentals of physics but also as a peace project, bringing scientists of many nations together in a peaceful enterprise. This concept connects firmly with what our scientific community is doing now in facilitating the Middle East synchrotron in Jordan and helping with the African Light Source project. The IUCr itself is directly active as a promoter of these with its [Light Sources for Africa, the Americas, Asia and Middle East Project \(LAAAMP\)](#), which it is conducting along with the International Union of Pure and Applied Physics under the auspices of the International Council for Science. Our IUCr Congresses also require free circulation of scientists, another vital ingredient for peace. We are striving to improve ourselves with respect to gender balance within all our activities; Bellamy in multiple places in his book emphasises the importance of this for societies striving for peace. As crystallographers we can then all take many direct roles as our contributions towards Peace in the World.

CRYSTALLOGRAPHY IN AFRICA

The journey of a young African scientist to crystallography

Mamoudou Diallo



Mamoudou Diallo (right) with his mentor (and Jedi Master), Claude Lecomte, at the IUCr-IUPAP-ICTP OpenLab Senegal in 2017.

I'm by no means an expert in crystallography but I want to tell of my experience for two reasons: first, as an acknowledgment to the IUCr for the [Crystallography in Africa initiative](#). Second, as an inspiration to the new generation of African crystallographers.

In his book *Crystal Structure Refinement, A Crystallographer's Guide to SHELXL*, Peter Müller wrote "The training of a crystallographer frequently reminds me of that of a Jedi Knight: the practical knowledge only goes from the master's mouth to the apprentice's ear and it can be difficult for the outsider or autodidact to become adept without a local guru's help". During the [Bruker/CCDC OpenLab Senegal, 5–10 October 2015](#) at Assane Seck Ziguinchor University, I was fortunate to meet and become a Padawan (Jedi Apprentice) of a very special Jedi Master whose main interest has been crystallography and its popularization in developing countries, Claude Lecomte, who had just completed his term of office as the Vice-President of the IUCr. I attended the OpenLab as an undergraduate student, looking for (among other things) fields on which to focus my graduate studies. I have found it and found so many tutors and lecturers willing to give me good advice about it. My interest in this fascinating world of crystals and crystallography stems from a lecture Professor Lecomte gave on X-ray crystallography (X-ray interaction with matter) and discussions we used to have at coffee breaks. I was very intrigued by those conversations and inspired by his personality and approach to crystallography. I remember asking him if

it would be possible to come to his laboratory at Lorraine University in Nancy, France, for PhD research about this subject of crystallography; he replied saying “Get done with your master’s first”. I finished my master’s one year later and applied for an international joint PhD between my local university (Assane Seck Ziguinchor University) and Lorraine University. This was my chance to become a young African crystallographer. In the beginning I started to read some crystallographic books and tried to grasp the fundamentals of the field but as Peter Müller said, crystallography is not an easy subject to be mastered from a textbook. The major event that shaped my career as a young student of crystallography was the bursary I was awarded to attend the Zürich School of Crystallography “Bring your own crystals”, 11–22 June 2017 at the University of Zürich, Switzerland. This school was crucial for me to gain insights into the fundamentals of X-ray crystallography. With the assistance of Tony Linden, Gervais Chapuis and Hans-Beat Bürgi, to name but a few, I was able to learn the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination. The enthusiasm for learning crystallography shown throughout the Zürich School by me and one of my colleagues (Marielle Agbahoungbata) overwhelmed the organizers so much that they mentioned it in their [meeting report in the IUCr Newsletter](#): “We were very impressed by two young scientists from Africa (Benin & Senegal), who were not only talented and keen to learn, but also eager to take their knowledge home in order to spread the word about crystallography in their region”. This was the same enthusiasm that we also showed at the [Joint Meeting of the Pan-African Conference on Crystallography \(PCCr2\) and The African Light Source \(AfLS2\)](#), 28 January–2 February 2019 in Accra, Ghana.



Mamoudou in discussion with Tony Linden at the Zürich School of Crystallography “Bring your own crystals” in 2017.

Another important crystallographic event I took part in was the [IUCr-IUPAP-ICTP OpenLab Senegal “Laboratory and synchrotron X-ray crystallography: applications to emerging countries”](#), 20 November–2 December 2017 in Ziguinchor, Senegal. It was during this OpenLab that I had the opportunity to meet other important figures of crystallography like Alessia Bacchi, former President of the European Crystallographic Association; Michele Zema, IUCr Executive Outreach Officer; and Nouredine Benali Cherif, from the Algerian Academy of Sciences and Technologies and Ecole Nationale Polytechnique, Constantine, Algeria. I was impressed by how approachable these professors were, and how they were

always happy to answer questions about relevant topics in crystallography. Another interesting aspect of this second OpenLab in Senegal was the opportunity it gave me to connect with numerous young scientists from all over Africa for potential future collaborations. For a way to stay in touch after the OpenLab, we initiated a WhatsApp group of young African crystallographers. This is today becoming a useful tool for dissemination of information related to crystallography between young African scientists and crystallographers across the continent. Another highlight event in my training career was the [fourth Summer School on Mathematical Crystallography](#), 3–7 June 2019, in Nancy, France. I'm very grateful to Massimo Nespolo who gave us a solid background in geometrical crystallography, which I deem essential for every student who wants to excel at this discipline. This School on Mathematical Crystallography has made a profound impact on me and on my outlook on crystallography and research in general. I think it's incredibly important for every young African scientist — and in particular women and underrepresented minorities in science — to have the opportunity to be involved in such an educative event.



Poster session at the MaThCryst Summer School in Nancy in 2019.

I'm happy that through these IUCr initiatives I had the opportunity to get to know about this fascinating field of crystallography and to share memorable times with renowned crystallographers. The two OpenLabs so far organized in Assane Seck Ziguinchor have allowed access to crystallographic knowledge in Senegal and have also started to open some possibilities for research in chemical crystallography. Two theses related to crystallography have been defended in the Chemistry Department and there are four doctoral theses being prepared in collaboration with the CRM² (Cristallographie, Résonance Magnétique et Modélisation) Laboratory at Lorraine University. Participating in OpenLabs and crystallographic schools is a unique chance to be surrounded by the best and well-known crystallographers and an excellent opportunity for getting inspired.

Nevertheless, despite IUCr's numerous outreach efforts, many challenges remain so far to be addressed, particularly in developing regions. Building capacities in these countries may be provided by extending further public awareness about the subject of crystallography, such as by providing more crystallographic schools, OpenLabs, workshops and lecture series. In addition to this, including

fundamental crystallographic courses in the academic curricular of developing countries would be another very effective way of providing educational opportunities that may impact students in their different fields of scientific study. Support also can be provided to some African young scientists by awarding bursaries to attend European crystallographic schools like the Zürich Schools of Crystallography, the MaThCryst Summer Schools in Nancy, France, or the AIC International Crystallography Schools in Italy. Facilities are also needed in Senegal as up to now, crystallographic experiments are not carried out on-site but abroad. This prevents access to instrumentation and does not enable us to perform hands-on experiments. In addition, international collaborations and strategic partnerships with representatives of local and regional scientific communities should be increased. This will lead to the implementation of national crystallographic associations in developing countries and facilitate the creation of the African Crystallographic Association (AfCA). As Dr Zema said during one of his lectures at the IUCr-IUPAP-ICTP OpenLab Senegal, quoting an African proverb, “If you want to go fast, go alone. If you want to go far, go together”. Now that the process of forming an African Crystallographic Association is imminent, let us all unite in a common effort to ensure that all the countries of the continent that are committed to science have a crystallographic association.



Mamoudou in discussion with Michele Zema at the IUCr-IUPAP-ICTP OpenLab Senegal in 2017.

Mamoudou Diallo is in the final year of a PhD in the Chemistry Department (Laboratoire Chimie et Physique des Matériaux, Groupe Matériaux Inorganiques GMI) of Assane Seck Ziguinchor University, Senegal. This is a joint PhD between Assane Seck Ziguinchor University and Lorraine University. He is working on the design and synthesis of lanthanide-transition metal molecular materials, under the supervision of Magatte Camara in Senegal and Mohamed Souhassou in France.

MEETING REPORT (IUCR SUPPORTED)

The 11th International Conference on Inelastic X-ray Scattering (IXS2019)

Yong Cai Mark Dean Ignace Jarrige



IXS2019 conference photo in front of the Charles B. Wang Center on the campus of Stony Brook University.

The [11th International Conference on Inelastic X-ray Scattering](#) (IXS2019) was held 23–28 June 2019 at Charles B. Wang Center on the campus of Stony Brook University, New York, USA. This conference series, which started in 1992, serves as the prime forum for the community to highlight the latest scientific and technical advances in inelastic X-ray scattering (IXS). This year it was attended by 148 registered participants from 16 countries: Germany, Japan, UK, France, Sweden, Canada, China, South Korea, Italy, the Netherlands, Taiwan, Switzerland, New Zealand, Finland, Austria and USA. The conference was hosted by the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory (BNL) and was organized by a Local Organizing Committee chaired by Yong Cai (NSLS-II), Mark Dean (BNL) and Ignace Jarrige (NSLS-II).

The conference began with an overview talk by John Hill, Director of NSLS-II, entitled “The past, present and future of inelastic X-ray scattering”. He highlighted the key advances of the field over the last 50 years and the enormous potential impacts in future developments. The scientific program that followed was organized into nine sessions covering science topics ranging from quantum, energy and functional materials to soft, glassy and biological materials, studies in the time domains and under extreme and *operando* conditions, the latest developments in novel IXS instrumentation, experimental approaches and theories, and the future of IXS with storage-ring upgrades and at new XFEL sources. Each session,

where appropriate, began with a plenary talk that introduced the topic with highlights from the latest results of the field. These included the following:

- Young-June Kim (University of Toronto, Canada) on Quantum Materials I
- Giacomo Ghiringhelli (Politecnico di Milano, Italy) on Quantum Materials II
- Olivier Delaire (Duke University, USA) on Functional Materials
- Wanli Yang (Lawrence Berkeley National Laboratory, USA) on Energy Materials & Catalysis
- David Reis (Stanford University, USA) on Time-Domain Spectroscopy
- Maurits Haverkort (Heidelberg University, Germany) on Theory
- Thomas Gog (Argonne National Laboratory, USA) on Future with Storage Ring based IXS
- Chi-Chang Kao (SLAC National Laboratory, USA) on Future with XFEL based IXS

They were followed by invited and contributed presentations in each session. A total of 40 invited and 14 contributed presentations were featured in the 5-day program, leading to many interesting questions and lively discussions. In addition, the poster sessions with 58 posters were very well attended and were extended into coffee breaks throughout the conference. Four of the posters contributed by young scientists were selected by a committee chaired by Nozomu Hiraoka (National Synchrotron Radiation Research Center, Taiwan) to receive the IXS2019 Poster Prize sponsored by the American Physical Society. The winners were as follows:

- Brett Leedahl (Max Planck Institute for Chemical Physics of Solids, Germany)
- Ekaterina Paerschke (University of Alabama at Birmingham, USA)
- Daniel Mazzone (Brookhaven National Laboratory, USA)
- Mirko Elbers (Technische Universitat Dortmund, Germany)

A special awards session was held on the last day of the conference to acknowledge the winners and for them to present their work.



IXS2019 Poster Prize winners award ceremony. Pictured L-R: Nozomu Hiraoka (Chair of Poster Prize Award Committee), Brett Leedahl, Ekaterina Paerschke, Daniel Mazzone, Mirko Elbers and Yong Cai (Chair of IXS2019).

Thanks to the IUCr sponsorship, two young scientists received IUCr Young Scientist Awards and also presented their work at the awards session. They were Jaeyun Moon of California Institute of Technology and Yao Wang of Harvard University, USA. Here is what they had to say about the opportunity provided to them by the IUCr:

Jaeyun Moon - "I would like to thank the IUCr for the support I received during IXS2019. During the conference, I learned a great deal about X-ray and neutron scattering instrumentation and its application in many different areas of research ranging from biological systems and soft matter to glasses and quantum materials. This conference also gave me opportunities to meet and socialize with a lot of professors, research scientists, and fellow graduate students and postdocs, many of whom I will be working with in the near future. I am really grateful to the conference organizers for the fruitful conference and IUCr for their support."

Yao Wang: "I want to express my gratitude again for the support of the IUCr Young Scientist Award, which offered me the opportunity to participate in the IXS2019 conference. This conference is a very important platform to exchange ideas about X-ray scattering with the theoretical and experimental communities. Especially, the IUCr award session allowed me to present my recent theoretical research on time-resolved RIXS spectroscopies. In addition, through discussions with other attendees, I was inspired by many novel ideas and advanced techniques, which are not even published yet. These discussions have motivated some of my future research directions."



IUCr Young Scientist Award ceremony. John Hill, Director of NSLS-II, presented the Award to the two winners: Jaeyun Moon (Caltech, left) and Yao Wang (Harvard, right).

The chair of the International Steering Committee, Arun Bansil (Northeastern University, USA), gave a nice summary talk to conclude the conference. All in all, this conference was a great success.

We would like to thank all our sponsors and exhibitors, including NSLS-II, Brookhaven National Laboratory, Stony Brook University, IUCr, American Physical Society, *Applied Physics Reviews*, NSLS-II User's Executive Committee (UEC), Huber, Kohzu, Incoatec, JETC, Sydor Technologies, X-Spectrum, Inprentus Precision Optics and Bestec, for all their support. The next IXS conference will be hosted by Diamond Light Source, Oxford, UK, in 2021.

MEETING REPORT (IUCR SUPPORTED)

32nd European Crystallography Meeting

Marijana Đaković



The 11th Max Perutz Prize was presented to Elspeth Garman (centre) at the Opening Ceremony by ECA President Udo Heinemann (right) and the chair of the Max Perutz Prize Committee and ECA Vice President Marijana Đaković.

The [32nd European Crystallographic Meeting \(ECM32\)](#) took place in the beautiful city of Vienna, Austria, from 18 to 23 August 2019, and gathered 1061 crystallographers from 48 countries, including more than 200 students and 76 exhibitors.



(l-r) Klaudia Hradil, Kristina Djinovic-Carugo and Ronald Miletich, Chairs of the ECM32 Organizing Committee, open the meeting.

The Opening Ceremony was held in the historic Main Building of the University of Vienna, the conference venue. This site, located within Vienna's historic centre, and with its numerous lecture halls and impressive ceremonial chamber rooms, offered a unique and historical flair during the conference. The meeting attendees were welcomed by Udo Heinemann, President of the European Crystallographic Association (ECA); Arndt von Haeseler, Dean of the Center of Molecular Biology and Director of Max Perutz Labs (a representative of the Rectorate of the University of Vienna); Johannes Fröhlich, Vice-Rector for Research of the TU Wien; João Alves, Vice-Dean of Faculty of Earth Sciences, Geography and Astronomy (UNIVIE); Veronika Somoza, Vice-Dean of Faculty of Chemistry (UNIVIE); Karlheinz Schwarz, National Committee for Crystallography of the Austrian Academy of Sciences; and Kristina Djinovic Carugo, Klaudia Hradil and Ronald Miletich, Chairs of ECM32. During the Opening Ceremony, the 11th Max Perutz Prize was awarded to Elspeth Garman (University of Oxford, UK), for her contribution to the field of macromolecular crystallography. In her award lecture, she addressed the development of methods for cryo-crystallography and methods for monitoring and mitigating radiation damage in protein crystals. The ceremony was accompanied by several musical interludes provided by the Pacher family brass septet Mission ImBRASSible.



Participants during the lunch break.

Over the four days of the conference, the attendees enjoyed an attractive scientific programme consisting of 48 microsymposia and 16 keynote lectures, and two poster sessions based on more than 780 submitted abstracts, covering the latest advances in crystallography and related sciences. The programme was launched by the plenary lecture 'Prokaryotic Cytoskeletons' given by Jan Löwe (MRC Laboratory of Molecular Biology, Cambridge, UK), and the attendees were then able to enjoy four vibrant days of exciting science, a number of lunchtime meetings (Crystallographic Software Fayre and a variety of sponsored luncheon workshops) and several well-attended social events.



The Conference Dinner at Schönbrunn Palace Orangery.

The Conference Dinner took place in the orangery of the famous Schönbrunn Palace, the main summer residence of the Habsburg Emperors, which accommodated over 300 attendees. The Young Crystallographers Mixer took place on the 6th Floor Rooftop Terrace of the TU Wien where over 70 enthusiastic participants had a chance to relax and make new friends with the help of a light informal dinner and DJ entertainment. The attendees had also an opportunity to enjoy famous classical music pieces by great Austrian composers, performed by the TU Wien Orchestra in the wonderful atmosphere of the Votivkirche, located close to the conference venue. Social events were complemented by the Viennese Waltz Dancing Course, taking place at the lunchtime breaks, and a number of organized excursions and tours, among which there were tours to MedAustron in Wiener Neustadt and to the Atominstitut of the TU Wien.



The organizers at the Conference Dinner.

After its successful launch at ECM30 in Basel, the Science Slam was organised again at ECM32. The best and most entertaining 3-minute presentation, determined by the loudest applause from the audience, received an award sponsored by Stoe & Cie GmbH.

At ECM32, the Alajos Kálmán Prize was awarded for the first time. The prize was established by the Hungarian Chemical Society and endorsed by ECA, and was awarded to Luigi Nassimbeni (University of Cape Town, South Africa).



IUCr Travel Award recipients at the Closing Ceremony.

The scientific programme was closed by the plenary lecture 'Quantum Crystallographic Studies of Advanced Materials' given by Bo Brummerstedt Iversen (Aarhus University, Denmark). At the Closing Ceremony, poster prizes were awarded to 16 young scientists (the list is available [here](#)). Besides the main conference, 15 well-attended satellite workshops were held at TU Wien:

- 26th *WIEN2K* Workshop
- X-ray Spectrometry
- Data Science Skills in Publishing – IUCr Committee on Data
- CCP4 Structure Solution Workshop
- MaThCryst Satellite Meeting
- Neutron Scattering and Imaging
- CrysAC Workshop – IUCr Commission on Crystallography in Art and Cultural Heritage
- IUCr and ECA High Pressure Workshop
- Young Crystallographers Satellite Meeting
- *Olex2* Workshop
- Total Scattering Analysis with *DISCUS*
- European Crystallographic Computing Forum – SIG-9
- Fixed Target Serial Crystallography
- Low Resolution Structure Determination with *Phenix*
- Crystal Engineering using the Cambridge Structural Database

ECM32 continued an important initiative, started at ECM31 in Oviedo, to provide a free child-care facility for children of in-advance registered attendees, and the meeting gathered a total of 1231 participants, including children, accompanying persons and volunteering students.

MEETING REPORT

22nd Heart of Europe Bio-Crystallography meeting

Michael Weyand



Universitätszentrum Obergurgl, venue for HEC22. Photo credit: Tiia Monto, [Creative Commons Attribution-Share Alike 3.0 Unported \(CC BY-SA 3.0\) Licence](#).

In mid-September 2019, the 22nd Heart of Europe Bio-Crystallography meeting (HEC22) with more than 110 participants from Austria, Czech Republic, Germany and Poland was held at the HEC record altitude of about 1.907 m in Obergurgl in the Ötztal valley, Austrian Alps. This familiar bio-crystallography meeting was organized by Klaus Scheffzek and co-workers from the Medical University Innsbruck. They were the superb hosts of about 22 high-level scientific student and post-doc talks, 10 company sponsor presentations and the new HEC group welcome talk by Ursula Neu (Charité – Universitätsmedizin Berlin, Germany). On the one side, the talks covered topics from solving protein expression and crystallization problems to presenting structural breakthroughs by serial crystallography and cryo-EM. And on the other side, presentations by suppliers described not only well-established but also new crystallographic tools and equipment.

Before the social networking tours took place, ranging from guided high-mountain hiking to following James Bond “Spectre” traces, the HEC Lecture 2019 was given by Nobel Prize winner Venkatraman Ramakrishnan, showing in a very personal manner the pitfalls and highlights of the ribosome structure elucidation story. He also presented the IUCr-sponsored HEC Prize for the most outstanding scientific presentation to Eliżbieta Wator (University of Kraków, Poland) for her exceptional scientific work on substrate recognition by deoxyhypusine synthase. Although at the periphery of the European

crystallographic heart, this meeting continued the more than two decade long HEC meeting tradition of an excellent platform for a common get-together of crystallographic beginners, experienced PIs and industrial suppliers.

The next HEC meeting (HEC23), organized by Clemens Steegborn from the University of Bayreuth, will take place on 24–26 September 2020 in Bad Staffelstein, Germany. More information can be found [here](#).

MEETING REPORT (IUCR SUPPORTED)

Celebrating CIF in practice

Serena C. TarantinoMichele ZemaBrian McMahon



The first Crystallographic Information Fiesta (CIFiesta), an international crystallography school of the Commission on Teaching of the Italian Crystallographic Association (AIC), was celebrated last 29 August to 3 September 2019 in Naples.

A *fiesta* is 'an event marked by festivities or celebration' (lexico.com), often characterised by energy, enthusiasm and joyful passion. So how on earth does it come to be appended to CIF, the acronym for that most dry of topics, the Crystallographic Information Framework? The School took on the challenge of using CIF to demonstrate the centrality of good practice in data management to the proper conduct of structural science. Wide in scope - from the collection and evaluation of experimental data through the publication of research findings to the dissemination of structural results in crystallographic databases - the School aimed to teach young researchers how (and why) to abide by its motto - 'know your data ... trust your data ... share your data'.

The venue was Naples, that gorgeous Mediterranean city in the shadow of Mount Vesuvius. The lecturers and tutors were from the local Institute of Biostructure and Bioimaging of the CNR, the wider ranks of the AIC Commission on Teaching, major structural databases, and representatives of no fewer than seven IUCr bodies.* The students (47% female and 53% male) were from locations as diverse as Italy, Albania, Algeria, Belgium, Benin, Brazil, Jordan, Morocco, Peru, Poland, Russia, Switzerland, UK and Uruguay.

To provide context, Simon Hodson, Executive Director of CODATA, gave an opening Keynote describing CODATA's efforts to promote Open Science through the FAIR principles (that data should be findable,

accessible, interoperable and reusable). Increasingly, grant proposals require an account of the scientist's proposed data management plan, and the growing demands from policymakers and from journals that scientific results should be reproducible highlight the responsibility of the scientist to analyse data critically, make it available to peer reviewers and subsequent researchers, and ensure that methodology and computational methods are published or described in full. Loes Kroon-Batenburg demonstrated how crystallography was fortunate in handling well defined and accurately measured data of many types (raw, processed and derived), yet pointed out the opportunities for coming to wrong or imperfect conclusions - through error, inexperience or, in the worst case, dishonesty. The importance of permitting critical reanalysis of experimental data in any assessment of a scientific result was emphasised in a video contribution by John Helliwell, Chair of the IUCr Committee on Data, who also highlighted the benefits of archiving raw experimental data towards this end. Brian McMahon, of COMCIFS and CommDat, then gave a historical account of the development of CIF, the IUCr's data characterisation and exchange standard, and showed how the large and growing number of CIF dictionaries covered all aspects of crystallographic research. It was under the umbrella of data definitions covered by the CIF programme that the students would spend the rest of the School solving, refining and ultimately publishing structures.



A collage of images from the School. Clockwise from top left: Simon Hodson delivers the opening keynote lecture; Luigi Vitagliano opens the structure solution tutorial to the macromolecular stream; Tom Blanton delivers the ICDD database tutorial; Loes Kroon-Batenburg delivers a plenary lecture; students grapple with a tutorial exercise; a team of students presents the results of their tutorial.

Uniquely (to our knowledge) the School had the ambition to generate primary research publications through collaborative work involving tutors and students on unpublished data sets. Following plenary lectures on data collection, evaluation and interpretation (James Hester, Loes Kroon-Batenburg), symmetry (Mois I. Aroyo) and the CIF paradigm (Brian McMahon, James Hester), the students split into two groups for tutorial sessions, one looking at a zinc coordination polymer, the other at conformational aspects of *Thermotoga maritima* arginine-binding protein (TmArgBP). In both groups, unpublished data sets were examined and critically assessed.

The small-unit-cell-parameter tutorial was designed by Michele Zema and Serena C. Tarantino in such a way that three teams of students each worked on a different XRD dataset that had been previously collected by Chiara Massera on the same crystal under different conditions. The coordination polymer structure was solved and refined using the software package *Olex2*, with expert guidance from the package maintainer Horst Puschmann, with Larry Falvello completing the team of tutors. The data analysis of the macromolecular structure, planned and coordinated by Luigi Vitagliano, Luciana Esposito and Rita Berisio, was conducted using *EVAL15*, again with the expert help of its author, Loes Kroon-Batenburg.

As with any real data set, limitations, imperfections and peculiarities provided opportunities to deepen the students' understanding of the actual physical structures giving rise to the experimental data. The highlight of the School was the students' presentations, in groups, of their own analyses and interpretations of the data and the structural models derived from it. Following the successful structure determinations, students had the opportunity to work with some of the IUCr journals' publication tools in the course of preparing the articles for submission, notably *checkCIF* for the pre-submission validation of the polymer, and *publBio*, a CIF-related authoring tool for the protein structure. ***The articles were accepted for publication in IUCrData and Acta Cryst. F, respectively [1, 2], in the case of the polymeric structure just in time for the Closing Ceremony.***



At the Closing Ceremony, Michele Zema announces that the first CIFIESTA article is accepted for publication in *IUCrData*. The reaction of the students is enthusiastic.

Following the challenging, stimulating and perhaps exhausting tutorial work (with students working late into a Sunday evening on their presentations), the final section of the School consisted of more hands-on tutorials and lectures in the processes of deposition and use of three major structural databases (Cambridge Structural Database, Protein Data Bank and the Powder Diffraction File). Once again there was a strong focus on data quality, for it is only in having large quantities of trustworthy results that the databases can fulfil their objective of driving further scientific discovery on the basis of their accumulated knowledge.

The aim of any School is to teach its students to become better scientists. In this respect, we have tried to provide a rigour and quality of teaching that is only to be expected from the AIC and IUCr. However, we have also tried to provide a slightly different perspective from most established Schools, one that links together the traditional hierarchy of components of understanding: data, information, knowledge and wisdom. In the School prospectus, we wrote that '*crystallographic **information** is the component that bridges the gap between raw experimental **data** and the global **knowledge** bases represented by the curated structural databases. It is typically thought of in terms of publications in the scientific literature, but in fact is more than that. It includes the characterisation and understanding of the raw data collected in an experiment, an account of the methods applied to process and analyse those data to*

infer a structure, and a quantification of the extent to which features of the model should be trusted or treated with caution. In an era when crystal structure determination is considered routine and is often largely automatic, a critical appreciation of the quality of the results is increasingly important. This school will teach students to respect their raw data, extract the most reliable information they can, and disseminate that information in a complete and verifiable manner. In this way they will contribute to the sum total of scientific knowledge with rigour and integrity.' The prospectus ended with the disclaimer '*crystallographic **wisdom** is outside the scope of this course*'. Watching the students progress through the course of the week, from their first exposure to the huge amount of care that must go into proper interpretation of experimental data (something often overlooked in the easy operation of modern instrumentation), through their growing awareness of what made one data set more reliable and usable than another, to their confident presentation of their structural investigations, we wonder if that last sentence should be omitted from future editions of such a School!

And did the event live up to its promise of a celebration? Let's hear what the students had to say ...

"When I arrived I knew nothing and when I left I knew enough!"

"CIFiesta was a great experience. I learned so many things. It was a pleasure."

"A fantastic learning experience, spanning basic to high-level theory. I really enjoyed the school."

"Stressful but fantastic experience!"

"The experience was positive in all aspects. The choice of alternating theory and practice was really effective! The printed booklet with all slides should be exported to all schools!"

"I really appreciated the tutorials, and even more the informal atmosphere which plays a great role in growing interesting discussions."

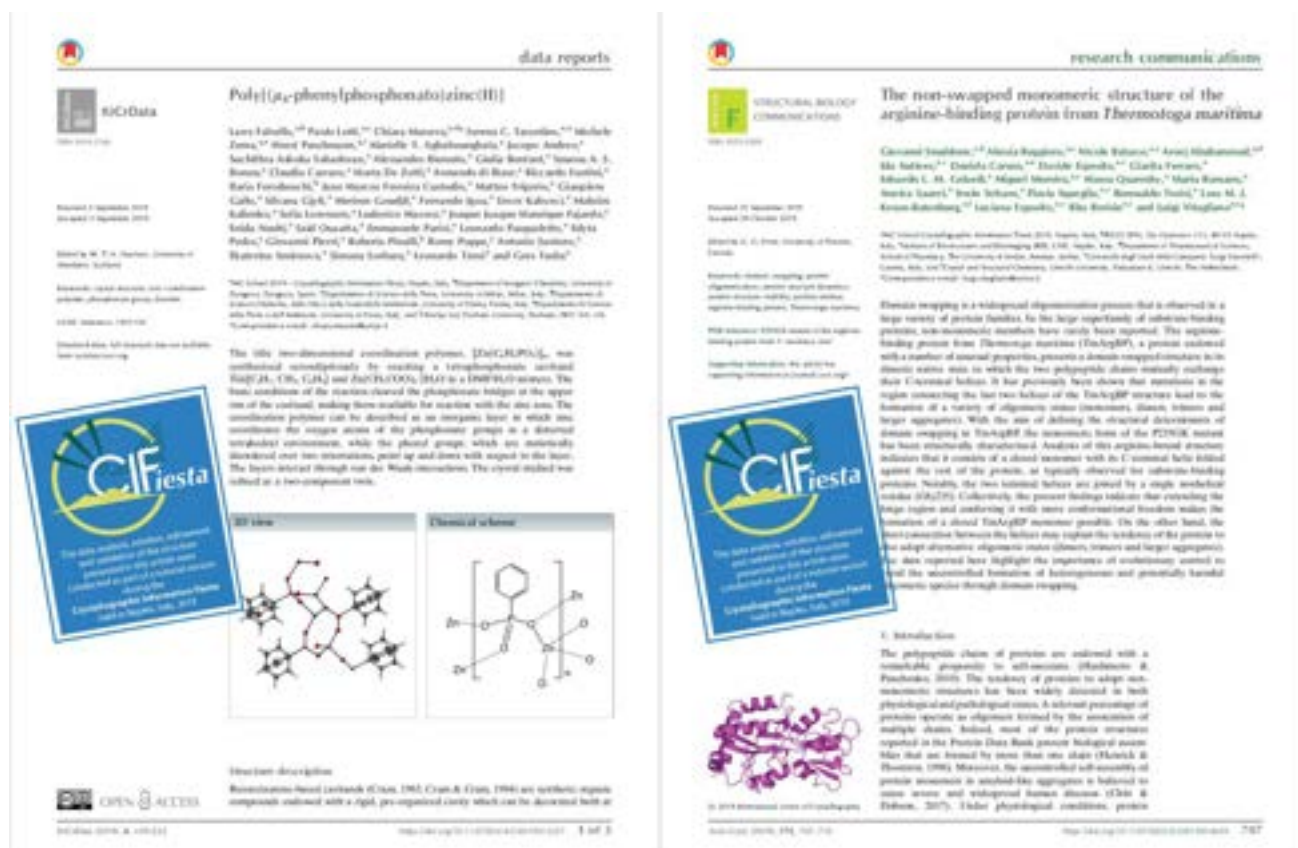
"The availability of school computers with pre-installed programs helps to pay full attention to the tutorial, not to handling software and hardware. Besides, the helping hand of several tutors' assistants contribute to the success of tutorials."

"I found the AICS2019 CIFiesta very successful, the academic activities were so rich and the computer-based tutorials have been very interactive. My experience with the school was AMAZING and I wish to take part in the next coming AIC schools."

"The school was excellent, the level was just right for me and for many of the students I have spoken with, practical sessions were short but super useful. All lecturers managed to generate an excellent environment of comfortability for discussions even though there was such an age (and ergo expertise) gap. Overall I loved it, so congratulations!!"

"This school was very useful for me. I learned many new things and deepened aspects that I already knew. The origin of students from different countries has made it even more fascinating. Congratulations on the organization."

"AICS2019 CIFiesta is very well organised. Thanks to the organising committee. I thank the IUCr for the financial support to allow my participation. I promise to be an expert in crystallography."



The first pages of the two articles published in *IUCrData* and *Acta Cryst. F* based on the activities of the tutorial sessions (small-unit-cell-parameter and macromolecular streams) conducted at the CIFiesta.

- [1] L. Falvello, P. Lotti, C. Massera, S. C. Tarantino, M. Zema, H. Puschmann, M. Y. Agbahoungbata, J. Andreo, S. A. Sahadevan, A. Bismuto, G. Bonfant, S. A. S. Bonou, C. Carraro, M. D. Zotti, A. di Biase, R. Fantini, I. Ferraboschi, J. M. F. Custodio, M. Frigerio, G. Gallo, S. Gjyli, M. Goudjil, F. Igoa, E. Kahveci, M. Kalienko, S. Lorenzon, L. Macera, J. J. M. Fajardo, E. Nushi, S. Ouaatta, E. Parisi, L. Pasqualetto, E. Pesko, G. Pierri, R. Pinalli, R. Poppe, A. Santoro, E. Smirnova, S. Sorbara, L. Tensi and G. Tusha (2019). *IUCrData*, **4**, x191222.
- [2] G. Smaldone, A. Ruggiero, N. Balasco, A. Abuhammad, I. Autiero, D. Caruso, D. Esposito, G. Ferraro, E. L. M. Gelardi, M. Moreira, M. Quareshy, M. Romano, A. Saaret, I. Selvam, F. Squeglia, R. Troisi, L. M. J. Kroon-Batenburg, L. Esposito, R. Berisio and L. Vitagliano (2019). *Acta Cryst. F*, **75**, 707–713.

* Lecturers included representatives of COMCIFS (the IUCr Committee on the Maintenance of the CIF Standard), CommDat (the Committee on Data), and the Commissions on Journals, *International Tables*, Mathematical and Theoretical Crystallography, Magnetic Structures and (ex officio) Crystallographic Nomenclature.

MEETING REPORT (IUCR SUPPORTED)

Fourth International School on Aperiodic Crystals

Olivier Pérez



The fourth edition of the International School on Aperiodic Crystals (ISAC4) took place from 8 to 14 September 2019 in Portbail in Normandy, France. Organized under the aegis of the Commission of Aperiodic Crystals (CAC) of the IUCr, it has been labeled a “thematic school” by the Institute of Physics of the CNRS and “Euroschoo” by the CmetaC network; it also received decisive support from the Normandy Region. Various other support, including from the IUCr and the French Crystallographic Association, made it possible to set up a scholarship system and to reduce the burden of enrolments in the overall budget of the school.

ISAC4 was organized within the VVF (Villages Vacances Familles) of Portbail to allow accommodation at the school. This unity of place was desired in order to encourage exchanges between participants and teachers. A total of 32 students (from France, Germany, Denmark, Sweden, UK, Italy, Slovenia, Croatia, Poland, Argentina, USA, Costa Rica and Japan) followed the theoretical lessons and tutorials given by nine international experts (from France, Israel, Germany, Czech Republic and Japan) in the field of aperiodic materials.

The school programme was constructed so as to gradually introduce the different concepts inherent in the field of aperiodic materials; tutorials allowing students to apply the concepts discussed were offered throughout the week. Thus, after a detailed introduction to aperiodic crystals (modulated structures, immeasurable composites, quasicrystals) placed in the context of classical crystalline compounds, the very particular case of quasicrystals was discussed by an approach using Landau theory. The formalism of the superspaces developed for the treatment of aperiodic phases was presented; this formalism

makes it possible, *via* the introduction of additional dimensions, to recover the three-dimensional periodicity absent in aperiodic compounds: physical space is then called "external space" or "parallel space" and the additional dimensions "internal space" or "perpendicular space". All of these notions were the subject of a tutorial during which the students were able to understand by geometric constructions the formalism of superspaces and the almost crystalline state by trying to achieve a Penrose tiling from *ad hoc* geometric pieces. All the concepts necessary for the structural determination of aperiodic crystals were then addressed: symmetry in superspace, indexing of diffraction diagrams with a tutorial that allowed students to work on real diffraction data from monocystals, and structural resolution theories for modulated phases and quasicrystals. At this stage the students were guided in the resolution of aperiodic structures during an afternoon. As the structural determination in superspace leads only to a model with $(3 + n)$ abstruse dimensions, the tools enabling comprehension of the final structural result for all novices were proposed. The dynamic aspects of the different types of aperiodic crystals were then described and a mode of excitation characteristic of the aperiodic order was defined: the phason. Finally, after a more theoretical description of the electronic properties of aperiodic surfaces and of the symmetry of quasicrystals, the aperiodic magnetic order was presented; a tutorial allowed the students to tackle the problem of solving an immeasurable magnetic structure.

These various lessons were "embellished" by various events such as a poster session allowing students to present their research work, an afternoon excursion with a guide to visit the harbor of Portbail and discover this Norman ecosystem, a gala dinner and a discovery of regional products. These social events aim to develop relationships between participants and create a bond in the community. A WhatsApp discussion queue "ISAC4" was also created by the students.

MEETING REPORT (IUCR SUPPORTED)

EXPO&more International Workshop

Angela Altomare



The EXPO&more International Workshop, organized by the Institute of Crystallography of the National Research Council of Italy, was held in Bari, a coastal town in southern Italy, from 30 September to 3 October 2019. The Workshop venue was the Videoconference room of the Polytechnic University of Bari.

The Institute of Crystallography of Bari has a long tradition of organizing meetings dedicated to the software developed by crystallographers of the Institute, for both single-crystal and powder diffraction.

The EXPO&more International Workshop was a four-day software fayre dedicated to the most recently developed versions of the open-source computer programs *EXPO*, *QUALX*, *OChemDb* and *RootProf*. Using diffraction data from polycrystalline materials, *EXPO* is devoted to crystal structure solution and *QUALX* to qualitative analysis for identification of the crystalline phase, one or more than one, contained in a compound. *OChemDb* is a web portal for assisting in the crystal structure determination process by retrieving information – from a suitably designed database of crystal structures already solved – on bond distances, bond angles, torsion angles, atom types and space groups. *RootProf* is an interactive general-purpose tool for fast processing of measurements from *in situ*, *operando* and/or multi-technique experiments.

The Workshop included both theoretical and computer sessions. The speakers, who were authors of the software, and the invited speakers, who were users of the software, presented the theoretical framework as well as the program workflow, the latest developments and examples of application. The participants

were familiarized with the computer programs during the hands-on sessions, also working on their own data.

The EXPO&more Workshop brought together 75 scientists (32 female and 43 male) coming from several countries all over the world (Nigeria, South Africa, Poland, Spain, France, Germany, Romania, Russia, Switzerland, Algeria, Morocco, Tunisia, UK, USA, Brazil, South Korea and Japan) and 4 continents, as well as from different research fields. It created full participation and great scientific interest. In particular, young scientists took advantage of the support from the direct discussions with the authors of the software, which were friendly and scientifically effective.

The Workshop enjoyed financial support from the Institute of Crystallography of the National Research Council (Italy), IUCr, Italian Crystallographic Association (AIC), Rigaku, PolyCrystalLine, *Crystals*, Assing, Excelsus Structural Solutions Company and Fondazione Puglia. The collaboration with Elettra Sincrotrone Trieste was also fruitful. The attendance of 21 young scientists was covered by sponsorship from the IUCr, AIC and Excelsus; 15 of them, financially supported by the IUCr, were celebrated during the Award Ceremony (see the photo below).



The EXPO&more Workshop was effectively conducted, spreading crystallographic knowledge and presenting methodological and computational tools able to successfully face several scientific purposes in the field of powder diffraction.

MEETING REPORT (IUCR SUPPORTED)

Hot Topics in Contemporary Crystallography 4

Ana Šantić



Presenters of the discussion-triggering presentations (l-r): Romualdo Troisi, Christine Touma, Nives Ivić and Vera Pfanzagl.

The fourth workshop [Hot Topics in Contemporary Crystallography \(HTCC4\)](#) held in Mlini, Dubrovnik, Croatia, 1–6 October 2019, was organized by the Croatian Association of Crystallographers and generously supported by Bruker AXS, JEOL and S.C.A.N. d.o.o. (golden partners), Aparatura d.o.o., Formulatrix, Rigaku, Dectris, *Crystals*, MiTeGen, the Croatian Ministry of Science and Education, the Croatian Academy of Science and Arts, the IUCr and the European Crystallographic Association. HTCC4 was entirely dedicated to structural biology with the programme comprising four hot topics on techniques and methods that go beyond classical crystallography: (i) XFEL (X-ray free-electron laser) (HT1), (ii) cryo-electron microscopy (HT2), (iii) nuclear magnetic resonance (NMR) in macromolecular structural research (HT3) and (iv) biomolecular *in-silico* simulations (HT4). Each topic was presented and discussed through an intense full-day programme of lectures and hands-on sessions conducted by the leading experts in the field.

HT1: Structure determination using XFEL (2 October 2019)

1. Henry Chapman, Center for Free-Electron Laser Science DESY, University of Hamburg, Germany.
2. Saša Bajt, DESY Photon Science, Hamburg, Germany.
3. Thomas White, Center for Free-Electron Laser Science DESY, University of Hamburg, Germany.

HT2: Cryo-electron microscopy (3 October 2019)

4. Jürgen Plitzko, Department of Molecular Structural Biology, Max Planck Institute of Biochemistry, Munich, Germany.
5. Carrie Berneky, Institute of Science and Technology (IST) Austria, Klosterneuburg, Austria.

HT3: Protein structure determination by NMR (4 October 2019)

6. Oliver Zerbe, Department of Chemistry, University of Zurich, Switzerland.

HT4: Biomolecular simulations (5 October 2019)

7. Franca Fraternali, Randall Centre for Cell and Molecular Biophysics, King's College, London, UK.
8. Chris Oostenbrink, Institute of Molecular Modeling and Simulation, University of Natural Resources and Life Sciences, Vienna, Austria.

The programme was additionally enriched with three invited lectures given by Zoran Štefanić (Ruđer Bošković Institute, Zagreb, Croatia) “Molecular visualization: scientific art and artistic science”, Udo Heinemann (Max-Delbrück Center for Macromolecular Biology, Berlin, Germany) “Crystallographic Studies of Nucleic Acid Sequence Readout by Proteins” and Areej Abuhammad (School of Pharmacy, University of Jordan, Jordan) “Structural studies on carbonic anhydrases: a crystal story from Jordan” as well as short presentations by the sponsor representatives: Yusuke Nishiyama (JEOL), Marcus Winter (Rigaku), Sacha De Carlo (Dectris) and Guillaume Brunetti (JEOL).

HTCC4 in numbers

Altogether, HTCC4 had 58 participants: 30 students, 9 lecturers, 7 organizers (two of them were also lecturers), 7 sponsor representatives and 7 accompanying persons. The participants came from 17 countries: Croatia (14), Austria (9), Germany (9), Slovenia (4), Switzerland (3), UK (3), Italy (2), Poland (2), Russia (2), Sweden (2), South Africa (2), Spain (1), France (1), Finland (1), India (1), Jordan (1) and Japan (1). The overall gender distribution of the participants was 45% female and 55% male.



HTCC4 participants.

Discussion-triggering presentations and best poster award

The HTCC4 programme contained two sessions intended especially for young participants to encourage them to present their research: discussion-triggering presentations and a poster session. Based on the quality of the submitted abstract, the potential of the abstract to trigger high-quality discussion as well

as the scientific background, four young participants (PhD students/postdocs) were selected to deliver short presentations:

1. Vera Pfanzagl (University of Natural Resources and Life Sciences, Vienna, Austria): “X-ray induced reduction of heme metal centers is protein-independent – implications for structural studies of redox sensitive proteins”
2. Christine Torma (University of Oulu, Finland): “Using nanobodies against CNPase as a crystallisation tool”
3. Nives Ivić (Ruđer Bošković Institute, Zagreb, Croatia): “Cryo-EM structure of the Imp7:Imp β :H1.0 complex”
4. Romualdo Troisi (Università di Napoli Federico II, Italy): “Human alpha-thrombin modulation by oligonucleotide aptamers: a molecular dynamics study”

The poster session contained 18 presentations, which were displayed during the entire duration of the workshop. The presented posters covered various topics within the field of structural biology. The *Crystals* best poster award, which focused on excellence in research, clarity of presentation, personal knowledge and understanding of the matter, was given to Radosław Pluta (Barcelona Institute of Science and Technology, Spain) for his work on “Structural basis for DNA recognition by FoxH1 pioneer transcription factor” authored by R. Pluta, E. Aragón, J. Cordero, P. Martín-Malpartida, L. Ruiz and M. J. Macías. The prize consisted of a certificate and an opportunity to publish a paper in *Crystals* or in the joint Special Issue with HTCC4 free of charge.



Winner of the best poster award, Radosław Pluta (left).

IUCr sponsorship

The IUCr generously supported HTCC4 enabling the Organizing Committee to allocate 11 bursaries to the utterly motivated students. All of them expressed their appreciation for the IUCr Young Scientist Awards bursary and stated their benefits from attending HTCC4. Some of their personal statements are given below.

Radoslaw Pluta, PhD student, Barcelona Institute of Science and Technology, Spain: “The IUCr Young Scientists Awards bursary that supported my participation in the Hot Topics in Contemporary Crystallography 4 – Structural Biology workshop gave me the excellent opportunity to learn from the top scientists in X-ray free-electron laser (XFEL) crystallography, single-particle cryo-electron microscopy (cryo-EM), cryo-electron tomography (cryo-ET), NMR in macromolecular structural research, and biomolecular *in-silico* simulations. The examples of particular systems studied with the presented methods and round table discussions helped me understand the complementarity between these methods and classical crystallography in contemporary research. By presenting my findings on the structural basis of DNA recognition by the FoxH1 pioneer transcription factor to the international scientific community I could engage in the exchange of ideas with both young and senior researchers and build networks with experts in complementary fields. Overall, this experience was valuable for the development of my career as a young independent researcher. Finally, I was happy to share the knowledge I grasped with my lab mates and colleagues at my Institute.”

Romualdo Troisi, PhD student, Università di Napoli Federico II, Napoli, Italy: “Receiving the IUCr bursary, which covered my accommodation costs, was very important for me. I could hardly have sustained the entire expense, considering the few funds available for PhD students in Italy. This course has been a great and unique opportunity to expand my knowledge in the field of structural biology, learning more about techniques that I do not currently use in my research activity and expanding my knowledge in the field of molecular dynamics simulations. Furthermore, it was very useful to present part of my work in the discussion-triggering presentation. It was my first oral presentation at an international conference. Thank you very much.”

Aleksandra Maršavelski, research associate, University of Zagreb, Croatia: “Attending HTCC4 was beneficial to me because I got detailed insight into structural methods NMR and cryo-EM. Namely, structures of many bio(macro)molecules that I use in my daily work are solved by using these methods. Therefore, being introduced to limits and pitfalls as well as advantages of these methodologies helped me to better understand the process of obtaining the structures. The most beneficial to me was a day dedicated to biosimulations. More precisely, interaction and discussion with Professor Oostenbrink helped me with my ongoing project and how to deal with one specific problem related to the relevancy of two possible rotamers of tyrosine.”

Ana Pavić, PhD student, University of Leeds, UK: “Attending the HTCC workshop this October in Mlini was a great experience overall and I really enjoyed this event! In my opinion it was very well organised, informative and engaging – meaning very successful and in a fantastic atmosphere. Lectures were interesting and informative on the particular subjects. Personally I made great use of the workshop – it not only solidified my knowledge about structural biology and exposed me to excellent lecturers, but it also enhanced my self-confidence as a research scientist. It was a pleasure to share my personal knowledge about membrane protein crystallography approaches. Furthermore, I found discussions with experienced international colleagues and professors helpful for my PhD project, as I came up with new ideas and approaches regarding my work. As my current PhD position has little funding for travel, this bursary was very important in enabling me to attend the workshop and reduce all costs. Thank you all – for offering me the bursary, for the effort to make this workshop happen, and for making me feel so welcome!”

Tamara Šmidlehner, post-doctoral researcher, National Institute of Chemistry, Ljubljana, Slovenia: “Receiving IUCr bursary was very helpful, otherwise I wouldn't probably attend the workshop. On the other hand, the workshop was highly beneficial for me, as I am fresh in this field of structural biology so the concept of the workshop gave a great overview of the methods used to determine the structure of proteins. Most of the lecturers were really good and they composed their presentations so that the basic background was given supported with case studies and advice on the planning of experiment and how to approach it. I liked the concept of the small-group workshop that definitely helped scientists to interact and discuss more easily.”

Marco Bardini, student, University of Parma, Italy: “I am still a young researcher, and I was one of the few HTCC4 attendees who had not yet started his PhD. For this and other reasons, I was honoured to receive an IUCr bursary to attend this conference and to be able to learn about so many different facets of how a contemporary scientist can tackle the problem of determining the structure and dynamics of biomolecules. The Universities in which I conducted my studies gave me a comprehensive education on the basics of crystallography and on the structural determination of materials and small molecules, but protein crystallography, as well as complementary techniques such as cryo-EM, were noticeably absent. This workshop gave me the opportunity to further my education in those areas and interact with research leaders in a field with which I was not overly familiar. The knowledge I acquired will be extremely useful once I start working on my PhD within the Marie Skodowska Curie Actions program, and I will never forget the friends I made during these intense, but rewarding, days in Mlini.”

In conclusion, HTCC4 was a successful workshop with highly motivated participants, enthusiastic lecturers, a vibrant atmosphere and good organization.

MEETING REPORT

Crystallography Symposium at STT45



A gathering of over 40 crystallographers, aspiring and experienced, was held recently in Chiang Rai in the north of Thailand as part of the 45th Congress on Science and Technology of Thailand (STT45). The full-day symposium was organised by Nongnuj Muangsins and Kuakarun Krusong (Chulalongkorn University) and Kittipong Chainok (Thammasat University), and was generously sponsored by Bruker Switzerland AG. Participants were drawn from the macromolecular and chemical crystallography communities. Along with conventional Oral and Poster Presentations, the Flash Presentation (3-minute talks/one slide) session was very popular. Siripak Jittirattanakul won the Bruker crystal award for the best Oral Presentation with the Bruker young crystallographer prizes awarded to Pakinee Srilaoong, Chana Panyanon and Siripak Jittirattanakul. Also, a very special mention must go to Purita Aroonchat, a pre-university scholar at Thammasat University, who won the book prize for the best Flash Presentation.



MEETING REPORT

PCG-SCMP Winter Crystallography Meeting

David KeenGoodwin Group



The grandly titled "Winter Crystallography Meeting" was inaccurately held at the very beginning of November at Milton Hill House near Abingdon, UK. This meeting incorporated the Winter Meeting of the Physical Crystallography Group of the British Crystallographic Association/the Structural Condensed Matter Physics Group of the Institute of Physics with the ISIS Crystallography User Group meeting and the Diamond Crystallography Group. In this context "Winter Crystallography Meeting" appeared remarkably succinct! Around 120 people attended, mostly from within the UK, to hear a wide range of talks very loosely within the remit of physical crystallography mainly, but not exclusively, with a central facilities flavour. The meeting ran over two days with the talks divided into five sessions.

The first session focused on structure-property relationships of a range of energy materials. The invited talks were given by Hamish Yeung (Birmingham) and Siân Dutton (Cambridge). Hamish showed the application of *in situ* X-ray diffraction as a central tool to study the crystallisation mechanism and kinetics of a series of metal-organic frameworks (MOFs) that can find their use in gas absorption and carbon capture, etc. For Cd-mixed ZIF-8, he showed how to use computational methods combined with elemental mapping to model particles with a core-shell structure, and how to verify these models by using XRD peak shapes. Siân gave an overview of her research on battery electrode materials with a unique perspective on how magnetic property measurements can assist in structure characterisation of materials with complex structures, particularly those with intricate stoichiometry and charge ordering. The contributed talks were given by Aron Summer (Warwick), Nicolas Flores-Gonzalez (Glasgow) and Ella Mara Schmidt (Oxford). Aron presented his work on how to use the Reverse Monte Carlo (RMC) method to model total scattering data on a series of nanocrystalline $\text{Ce}_{1-x}\text{Zr}_x\text{O}_2$ materials used in catalysis.

Nicolas talked about tuning the lattice polarisability using different halides and its effect on the Li conductivity in LiAlX_4 ($X = \text{Cl}, \text{Br}, \text{I}$), a solid electrolyte for batteries. Ella introduced her superspace method with the help of a "superspace piano" to study occupational and displacement disorder in crystalline materials using single-crystal diffuse scattering.



Speakers: (L-R) Jacinthe Gamon, Abby Haworth, Martin Dove, Alice Bumstead and Chloe Fuller presenting their talks.

The second session started with invited speaker Eddie Cussens (Sheffield) "Throwing crystallography, spectroscopy and the kitchen sink in (magnetic) frustration" at a number of double perovskites, with the complex magnetic behaviour being studied over different timescales using different techniques. Jonathan Bulled (Oxford) continued the theme of magnetic frustration in the second presentation, this time on the trillium lattice in a $\text{NaMn}(\text{HCO}_2)_3$ MOF; he highlighted some potential applications of frustrated magnets, for example as magnetocalorics. Following this were a couple of talks on lithium conducting materials. First, Abby Haworth (Durham) demonstrated the use of nifty nuclear magnetic resonance (NMR) experiments to detect Li and Na ion mobility in Li-stuffed garnet, and how Na doping affects the ionic conductivity. Next up, Jacinthe Gamon (Liverpool) showed how a computational exploration of the Li-Al-S phase field resulted in the discovery of a new sulfide, Li_3AlS_3 , and also how structural studies revealed the Li conductivity mechanism. More MOFs followed, with Daniel Bowron (ISIS) presenting the use of total scattering experiments to study the structure of liquid O_2 confined in ZIF-8 as a function of gas pressure, and how this differs from pure O_2 . The session finished with Noah Waterfield-Price (Oxford) giving the Malvern Panalytical Thesis Prize Talk about the domain structure in multiferroic BiFeO_3 . It was a fantastic recount of how neutron and X-ray diffraction, along with photoemission electron microscopy, were used to identify magneto-structural domains and how the domain structure is coupled to polarisation in the material.

The session was followed by a bustling evening poster session, with 40–50 posters squeezed into the room. Prizes were awarded at dinner, just before the now traditional sticky toffee pudding dessert, to Emily Reynolds and Philip Welch (both Oxford) for their poster presentations on innovative MOF synthesis and disordered magnetic states in CsCoCl_3 , respectively.



Prize winners: (L-R) Noah Waterfield-Price receiving the Malvern Panalytical Thesis Prize from Paul O'Meara (Malvern Panalytical), Philip Welch and Emily Reynolds receiving poster prizes one minute apart from Helen Playford (ISIS), and Anna Herlihy with her cider-themed poster prize presented by Steve Hull (ISIS) in memory of Sten Eriksson.

The following morning, the third session remembered Sten Eriksson, who led the long-running collaboration between the Swedish scientific community and ISIS. He sadly passed away in December 2018. In his memory an additional poster prize was awarded to Anna Herlihy (Warwick/ISIS) for her poster entitled "Pressure-induced phase transitions of the improper ferroelectric $\text{HgMn}_7\text{O}_{12}$." The talks presented in the session covered a large variety of materials and research techniques. Paul Attfield (Edinburgh) introduced double double perovskites and the possibility of triple double perovskites using high-pressure synthesis to increase the accessibility of interesting physical properties by cleverly tuning composition. Steve Thompson (Diamond) took the audience on an interstellar journey to the analysis of interstellar dust and its replication in the laboratory. The intercalation of ammonia and lithium was discussed in Machteld Kamminga's (Oxford) talk on layered chalcogenides. The session was closed by Lee Brammer (Sheffield) introducing some flexible, dynamic MOFs where the breathing behaviour is solvent dependent and can accommodate different activated states.

The fourth session explored a range of exciting dynamic properties of materials. Mark Warren, beamline scientist from I19 at Diamond, demonstrated how they are pushing the boundaries of pump-probe experiments looking at excitations in ambidentate linkage isomers. Chloe Fuller (Durham) reported total scattering measurements exploring the effect of vacancies and doping in the ion-conducting oxide $\text{Sr}_2\text{ScGaO}_5$. With Johan Cedervall (Stockholm/ISIS) we were treated to the complexity of the high-entropy alloy phase diagram for AlCoCrFeNi , which is dependent on cooling rate, heating rate and particle size: how can we control these to maximise its favourable mechanical properties? Martin Dove (Queen Mary) explained the astonishing and counterintuitive pressure-induced softening in ScF_3 and attributed this to the unusual flexing of the ScF_6 octahedra. In exploring the melting behaviour of two compositionally similar but structurally distinct ZIFs, Alice Bumstead (Cambridge) revealed that whilst individually one melts and the other does not, the former can act as a solvent to assist the melting of the latter. David Keen (ISIS) then rounded off a fantastic session by using a study of the hydrogen disorder in the mineral hydrogrossular to highlight the intricacies of analysis and interpretation of neutron and X-ray total scattering.



Various: (Clockwise from top) Group photo with autumn colours, Steve Hull (ISIS) clearly happy with the choice of dessert at dinner, the packed poster session, and Emily Reynolds (Oxford) still delighted with her winnings (with Lewis Owen, Cambridge).

The four talks in the final session also covered an eclectic mix of subjects. Iain Oswald (Strathclyde) described how pressure can be used to recover metastable phases of small molecules such as paracetamol and caprolactum. John Claridge (Liverpool) aptly subtitled his talk, "What has superspace ever done for us?" with "how I learned to stop worrying and love the modulations" and Stephen Dodsworth (Sheffield/Diamond) showed us how the character of the breathing mechanism in MOF SHF-61 can be changed post-synthesis. The final talk of the meeting was given by Bob von Dreele (Argonne). He gave a presentation on GSAS-II, his Rietveld refinement code, and how it can be used to determine magnetic structures. In his introduction he reflected that his original GSAS code was borne out of work he did in the UK 47 years ago; GSAS-II now has 100 000 lines of Python code and he has returned to the UK for an extended visit to ISIS and Diamond to continue its development.

IUCR CONGRESS

Preparation and promotion of the 25th IUCr Congress in Prague

Radomír Kužel Ivana Kutá Smatanová



Congress Chair Radomír Kužel welcomes visitors to the joint IUCr/Congress booth at the 2019 MRS Fall Exhibit.

After having all 3 plenary and 36 keynote lectures confirmed by the speakers, we have focused on the preparation of 104 regular microsymposia by inviting all co-chairs in collaboration with International Programme Committee (IPC) members. With respect to the original proposal from the IPC Prague meeting in May 2019, one session was replaced by "Recent advances in instrumentation" and one significantly renamed; the others remained as suggested. Currently we are missing five co-chairs only. There are still some slots in the special programme in the 9th parallel session.

The list of workshops and satellites has been enlarged as follows:

- Computing school, 17–22 August in Nové Hradky, South Bohemia
- Electron crystallography school, 19–22 August in Tábor, South Bohemia
- Small-angle scattering workshop, 19–21 August, probably in Kutná Hora
- Macromolecular Machines in Biomedicine: Structure, Dynamics, and Evolution workshop, 21–22 August, Prague Congress Centre
- Methods of Structural Biology, 18–21 August, Vestec near Prague

- School on Aperiodic Structures of Quasicrystals, Magnetic Materials, Minerals and Molecular Compounds: State of the Art in Structure Solution and Refinement workshop, 21–22 August in Prague
- 3rd IUPAC-ICSU Workshop on Crystal Engineering, 21–22 August in Prague
- TOPAS workshop, 21–22 August in Prague
- ICDD workshop, 22 August, Prague Congress Centre
- GISAXS workshop, 22 August, Prague Congress Centre
- XAFS workshop, 22 August, Prague Congress Centre
- School on electron PDF, 30 August–1 September, probably Kutná Hora

We continue to promote the Congress and shared the IUCr booth at the 2019 MRS (Materials Research Society) Fall Meeting from 2 to 6 December in Boston, MA, USA. We could see there that several important materials science topics have also been included in IUCr2020. We also hope to integrate the exhibition in the conference in a better way as it will be right in the centre and all coffee breaks and lunches will be served there. Basically, each participant will have to go through the exhibition area.

We have signed up main exhibitors and sponsors. ICDD has confirmed bronze sponsorship and Malvern Panalytical decided to go for gold. However, we are still waiting for several traditional exhibitors as well as some new ones.

All people interested are encouraged to register at www.conftool.com/iucr2020. The system will be used for everything connected with abstract submission, bursary applications, registrations (congress, workshops, events, trips) and payments. Currently, a nearly full detailed schedule of the conference is available there.

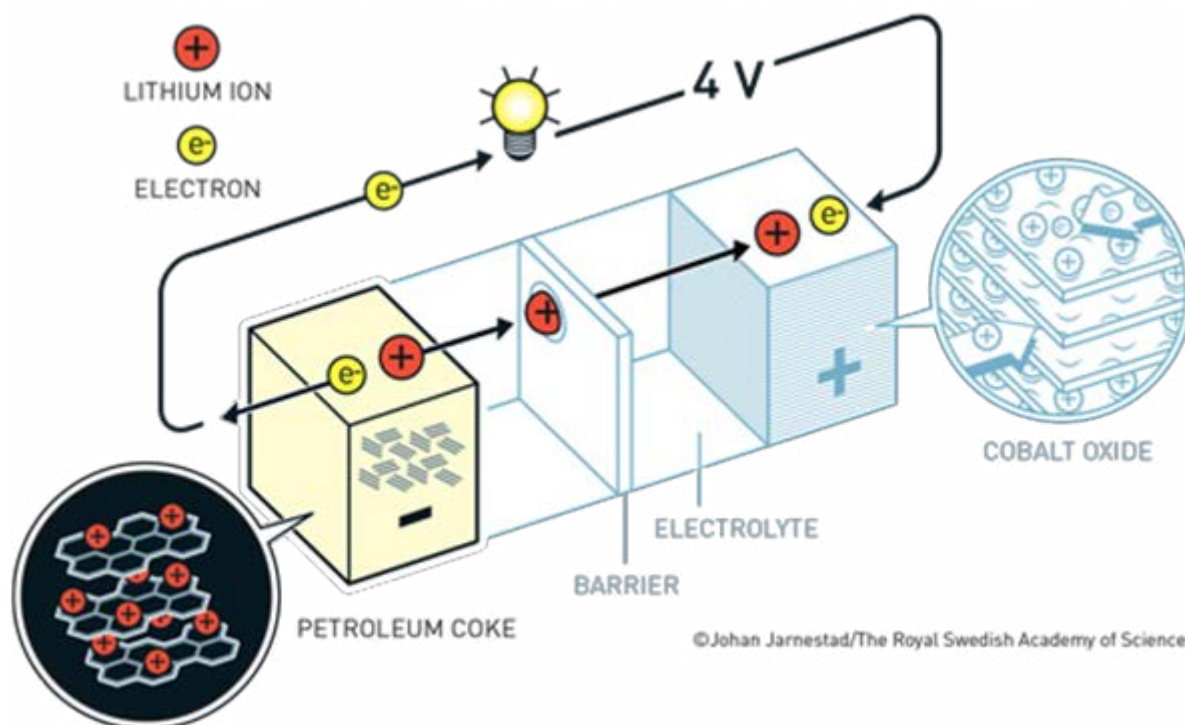
Finally a few important deadlines should be noted:

- applications for bursary – **end of February 2020**
- submission of abstracts to be considered for lectures in sessions – **31 March**
- early-bird registration – **15 May**.

The basic standard early-bird fee has been fixed at 620 EUR taking into account all the IUCr conditions, the 7-day duration of the congress (as it is held only once every three years, the agenda is rather full) and the decision to include lunches in the fee (as required by companies and local conditions).

AWARDS AND PRIZES

Nobel Prize in Chemistry 2019 awarded for development of lithium-ion batteries



The Royal Swedish Academy of Sciences has decided to award the [Nobel Prize in Chemistry 2019](#) to John B. Goodenough (University of Texas at Austin, USA), M. Stanley Whittingham (Binghamton University, State University of New York, USA) and Akira Yoshino (Asahi Kasei Corporation, Tokyo, Japan, and Meijo University, Nagoya, Japan) “for the development of lithium-ion batteries”.

Lithium-ion batteries have revolutionised our lives since entering the market in 1991. They are lightweight, rechargeable and powerful, and are used globally to power portable electronics - everything from mobile phones and laptops through pacemakers to electric vehicles. They can also store significant amounts of energy from renewable sources such as solar and wind power, making possible a fossil-fuel-free society.

The foundation of the lithium-ion battery was laid during the oil crisis in the 1970s. Stanley Whittingham worked on developing energy technologies that did not rely on fossil fuels. He started to research superconductors and discovered an extremely energy-rich material, titanium disulfide, which can intercalate lithium ions and which he used to create an innovative cathode in a lithium battery. The anode was partially made from metallic lithium, which has a strong drive to release electrons. The resultant device's potential was just over 2 V but the metallic lithium made the battery too explosive to be viable.

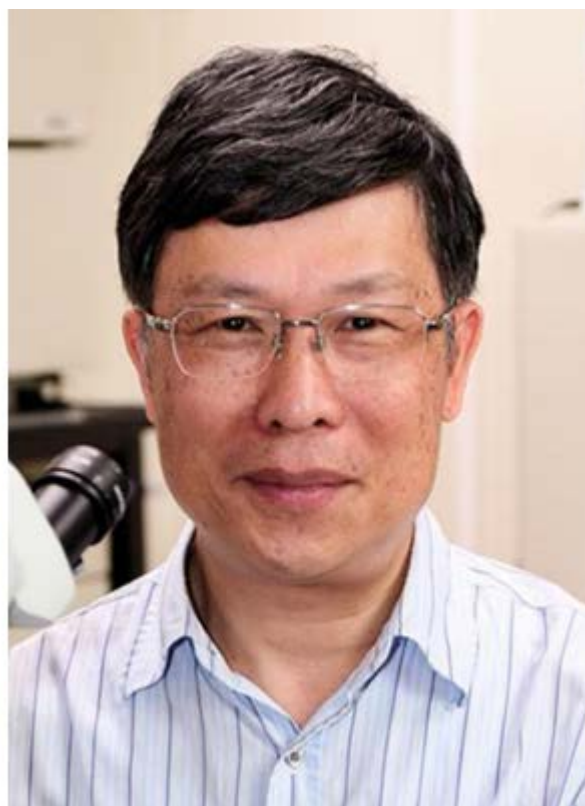
John Goodenough predicted that the cathode would have even greater potential if it was made using a metal oxide instead of a metal sulfide. After a systematic search, he demonstrated in 1980 that cobalt oxide with intercalated lithium ions can produce as much as 4 V. This was an important breakthrough and would lead to much more powerful batteries. With Goodenough's cathode as a basis, Akira Yoshino created the first commercially viable lithium-ion battery in 1985 (illustrated). Rather than using reactive

lithium in the anode, he used petroleum coke, a carbon material that, like the cathode's cobalt oxide, can intercalate lithium ions. The result was a lightweight, hardwearing battery that could be charged hundreds of times before its performance deteriorated. The advantage of lithium-ion batteries is that they are not based upon chemical reactions that break down the electrodes, but upon lithium ions flowing back and forth between the anode and cathode.

See the winners' research in IUCr journals [here](#).

AWARDS AND PRIZES

Studies of enzyme systems rewarded with the Aminoff Prize



Douglas Rees (left, photo credit: Caltech) and Jian-Ren Shen (photo credit: Okayama University).

The Royal Swedish Academy of Sciences has awarded the Gregori Aminoff Prize in Crystallography to Douglas Rees (California Institute of Technology, Pasadena, CA, USA) and Jian-Ren Shen (Okayama University, Japan) for *“their fundamental contributions to the understanding of biological redox metal clusters”*. The award ceremony and commemorating lecture will take place at the Academy’s annual meeting held in Stockholm on 30–31 March 2020.

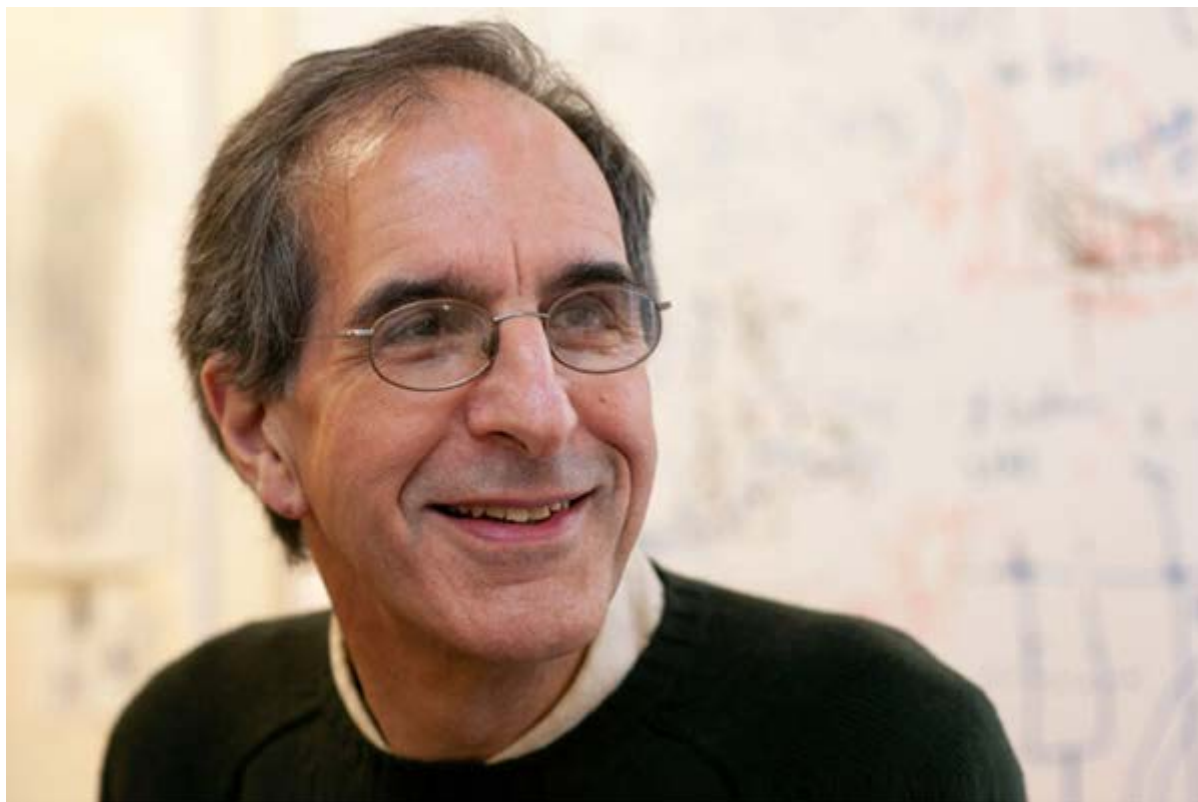
Jian-Ren Shen has studied a photosynthesis enzyme in plants and photosynthetic bacteria, called photosystem II, while Douglas Rees has studied nitrogenases, which fix atmospheric nitrogen and are found in some bacteria. However, studying these two enzyme systems is challenging. Both systems transfer electrons between different molecules using metalloclusters to temporarily store the electrons. In photosystem II this is a cluster of manganese ions and in nitrogenase it is usually iron. The X-ray radiation used in the study of these systems’ structures tends to change the oxidation state of the metal ions, which means the image produced is not always the same as the way enzymes look in their natural state. Nitrogenase has another difficulty, as the entire system is oxygen-sensitive and must be protected at every stage of the purification and crystallisation process.

For photosystem II, one way of removing the problem is to use short pulses of high-intensity X-ray radiation. This allows enough information about the structure to be collected during one pulse. No redox processes can take place in the short duration of the pulse, and the information from the experiment thus describes the undamaged system.

Jian-Ren Shen and Douglas Rees lead research groups that have succeeded in studying numerous different states in enzymes, which has led to an understanding of how nature drives photosynthesis and fixes atmospheric nitrogen using enzymatic processes.

The Gregory Aminoff Prize rewards a documented individual contribution to the field of crystallography, and has been awarded to Swedish and foreign researchers since 1979. The prize amount is SEK 120,000. More information is available [here](#).

OBITUARY

Cyrus Chothia (1942-2019)

Cyrus Chothia. © MRC Laboratory of Molecular Biology

Cyrus Chothia, former Group Leader and until recently emeritus scientist in the LMB's Structural Studies Division, died on 26 November 2019. Cyrus pioneered the use of computational methods to study the structure and function of proteins, and the evolution of genomes, which led to the birth of structural bioinformatics and computational genomics. His collaborations with several scientists, both at the LMB and elsewhere, helped to develop a wide variety of principles and computational methods, including developing a classification system of protein structures. He was an inspiration to many, particularly in the field of bioinformatics, and much admired by friends and colleagues.

"At the LMB, and throughout the world, Cyrus' influence, which he preferred to exert through quiet determination, was profound and long-lasting. The successes of the genomics and structural biology revolutions are unthinkable without Cyrus' contributions," said Jan Löwe, Director of the LMB.

Cyrus was born on 19 February 1942. He studied chemistry at the University of Durham, graduating in 1965 and then undertook an MSc in crystallography at Birkbeck College London. He completed his PhD, under the supervision of Peter Pauling at University College London, on the structure and function of the neurotransmitter acetylcholine in 1970, before arriving as a postdoctoral researcher at the LMB.

In 1973 Cyrus undertook a 'scientific grand tour', spending time with Fred Richards at Yale, Michael Levitt at the Weizmann Institute and Joel Janin at the Institut Pasteur in Paris. With Michael, he developed the "all- α , all- β , α/β and $\alpha+\beta$ " classification of protein structures. With Joel, he determined the principles that underlie protein-protein recognition and produced models that explain how secondary structures pack in proteins. These principles have been instrumental in interpreting the molecular basis of various diseases.

Cyrus returned to England in 1976 and for the next 14 years was attached to both the University College London and the LMB. Between 1980 and 1990 he was the EPA Cephalosporin Fund Senior Research

Fellow of the Royal Society. With colleague Arthur Lesk, he showed that proteins adapt to mutations by changes in structure, described the mechanisms that transmit information between distant sites in proteins and demonstrated that there is a small repertoire of main-chain conformations for immunoglobulin hypervariable regions and that those present in an antibody can be predicted from their sequence.

In September 1990, Cyrus became a Group Leader at the LMB. In 1992 he proposed that most proteins are built of domains that come from a small number of families. He collaborated with Alexey Murzin, Steven Brenner and Tim Hubbard to create the [SCOP database](#), a periodic table for all known protein structures, and with Julian Gough to create the SUPERFAMILY database, which uses hidden Markov models to identify protein sequences that are related to those with known structures.

Cyrus' innovative approach in applying his understanding of protein structures to completely sequenced genomes of organisms provided new insights into cellular systems. His work on eukaryotes showed that the number of members in the ~200 superfamilies, of the 1,200 that were known, correlates with the complexity of the organisms in which they occur. The increases in these superfamilies play a major role in increasing biological complexity, which is fundamental in generating the diversity of life forms.

"It is a great loss to the scientific community. Cyrus' contributions shaped how scientists approach biological questions with the use of data. He pursued this bold and unconventional path of enquiry to study structures and genomes at a time when it was unknown that data driven approaches could have such an impact on our understanding of organisms. For many of us, he was also an inspiring mentor," said M. Madan Babu, a group leader at the LMB.

Cyrus was elected to EMBO in 1998 and became a Fellow of the Royal Society in 2000. In 2015, he was awarded the highly prestigious international Dan David Prize and the International Society for Computational Biology (ISCB) Senior Scientist Accomplishment Award, both for his work in the field of bioinformatics. He has long been recognised as a leader in computational biology and bioinformatics and has mentored over 21 scientists (19 PhD students and 2 postdocs) during his career, several of whom have gone on to become leaders in the field of bioinformatics.

This obituary has been republished from the [MRC Laboratory of Molecular Biology website](#).

OBITUARY

Catalina Ruiz-Pérez (1957-2019)

Pilar Gómez Sal



It is with great sorrow that we report that our colleague Catalina Ruiz-Pérez passed away on 8 August 2019 at the age of 62.

Catalina Ruiz-Pérez was born in Valencia, Spain, in 1957 and she was Full Professor of Applied Physics in the Department of Physics at Universidad de La Laguna in Tenerife, Spain, since 2000. She was Director of the X-ray and Molecular Materials Laboratory at that University, where she served as Director of the Physics Department from 2004 to 2006 and as Vice-chancellor for Research and Knowledge Transfer from 2011 to 2014.

During her scientific career, Professor Ruiz-Pérez published over 250 research papers and book chapters, most of them in the field of crystal structure-property relationships in molecular materials, particularly in molecular magnets and crystal engineering. She also served in national and international scientific societies. For instance, she was Vice-President of the Nanoscience and Molecular Materials Group of the RSEQ (Real Sociedad Española de Química) from 2005 to 2010. She was a member of the Board of the Group of Crystallography and Crystal Growth (GE3C) of the RSEQ and RSEF (Real Sociedad Española de Física) since 1992, and acted as Vice President until 2015. She actively participated in the EIP (European Innovation Partnership) on Water, an EU Innovative Project. She was an organizer of the IUCr Congress in Madrid 2011.

In the field of International Cooperation, she was appointed Advisor in Research and Development of the CONCITEC (National Council for Science and Technology) and the Direction of Research of the ANR (Asamblea Nacional de Rectores) of Peru. She received several awards including the Canarias Award of Research and Innovation in 2017.

She will be sorely missed by her many friends and colleagues in the crystallographic community. Our thoughts and our warmest sympathies go to her husband, daughters and family.

IUCR SUPPORTED EVENTS

IUCr supported meetings

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



**11th Oct 2026 - 16th
Oct 2026**
Indaba10

Skukuza, Kruger National
Park, South Africa



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

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

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

	Indaba10 South Africa 11th Oct 2026 - 16th Oct 2026
	Synchrotron Radiation: Science, Knowledge, Innovations, Future (SKIF-2026) Russian Federation 18th Oct 2026 - 23rd Oct 2026
	CCP-EM/Diamond Icknield Workshop United Kingdom 9th Nov 2026 - 13th Nov 2026
	Instruct-ERIC hands-on workshop on Advanced cryo-FIB-SEM methods Germany 9th Nov 2026 - 13th Nov 2026
	Crystal36-AXAA 2026 Meeting Australia 26th Nov 2026 - 2nd Dec 2026
	African Materials Research Society (AMRS 2026) Kenya 5th Dec 2026 - 10th Dec 2026
	Joint Polish-German Crystallographic Meeting 2027 Germany 15th Feb 2027 - 18th Feb 2027