Crystallography News

British Crystallographic Association

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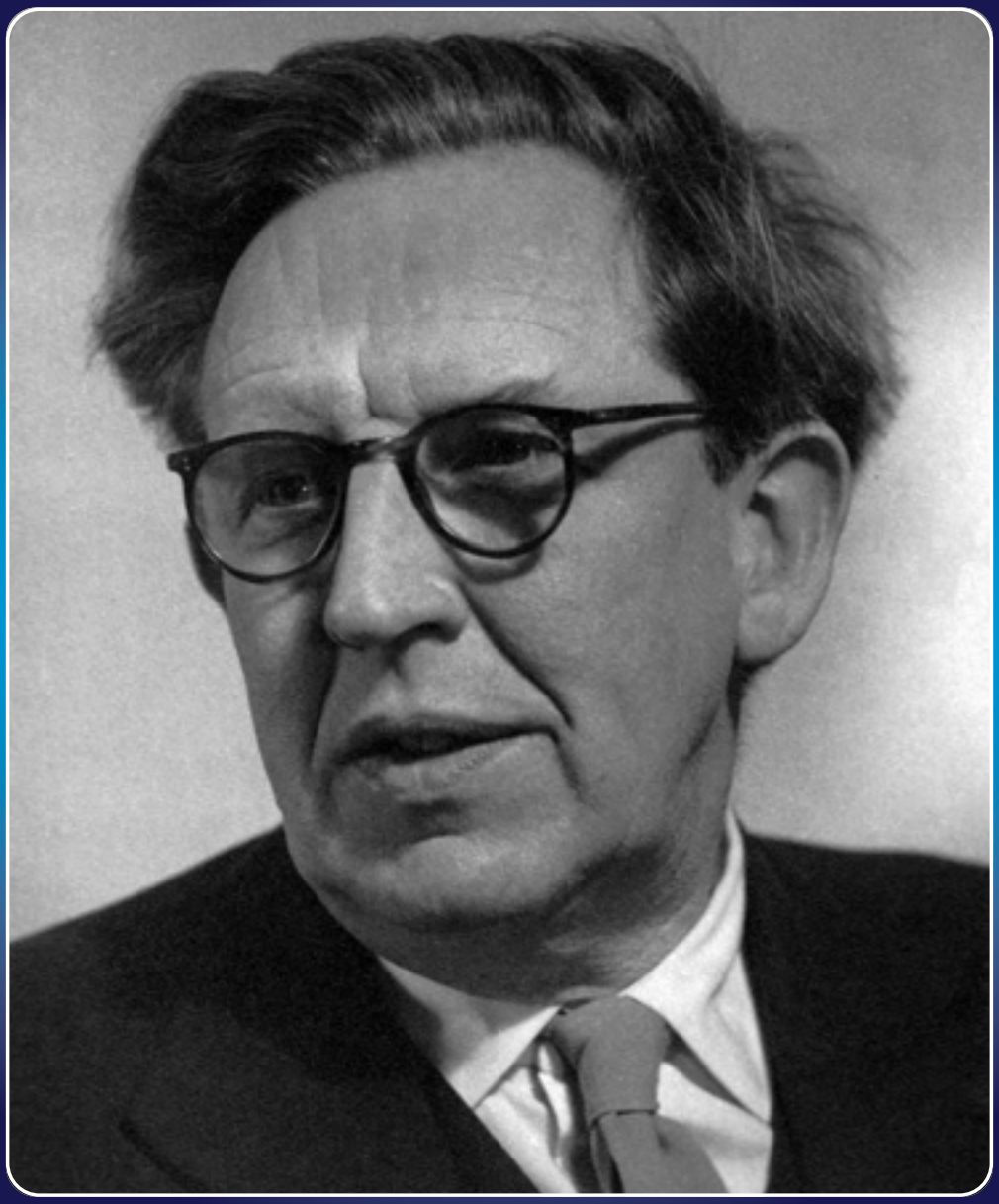

John Desmond Bernal 50th Anniversary

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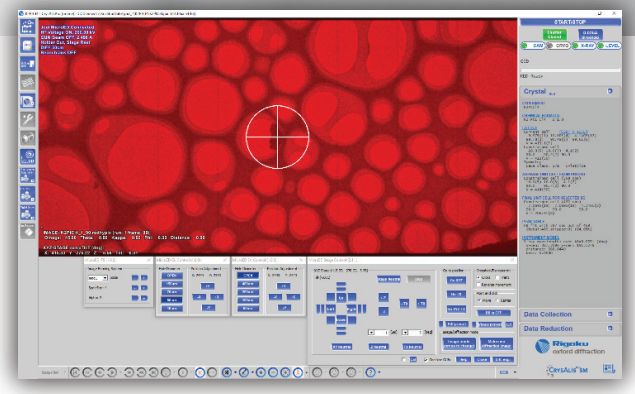

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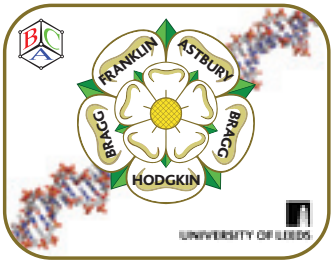

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the December 2021 issue are sent to the Editor to arrive before 25 October 2021.

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This month's cover:

John Desmond Bernal by Henry Grant (courtesy S. Jane Bernal).

From the President

WELCOME to the September issue of the BCA's Crystallography News and my second (of twelve) columns – not that I'm counting them down already.

As this issue lands on your doormat or email inbox, the first meeting of BCA Council since the Spring Meeting will be taking place. Amongst other things, we will be discussing communications and outreach projects and reflecting on news from the **IUCr Congress and General Assembly** in Prague. At the time of writing, the IUCr conference is yet to take place, but it seems likely that there will be very few in person delegates from the UK due to travel restrictions. The meeting is in a hybrid format, mixing real and virtual delegates, speakers and posters, and includes plenary talks from recent BCA Prize Lecturer **Clare Grey** and BCA Founder Member **Olga Kennard**. I look forward to virtually attending both the scientific talks and – because the BCA is the national adhering body to the IUCr – as part of the UK's delegation to the General Assembly. Reports from the meeting will be included in the December issue.

Next year will be 40 years since the founding of the British Crystallographic Association. Over the years we have digitized some historical documents of the BCA and placed them online, for example the signatures of the original Founder Members can be seen at **https://crystallography.org.uk/membership/founders/**. However, a lot more of it remains in boxes of minutes and old editions of *Crystallography News* in the corner of my office and it seems timely to endeavour to organise and make some of this material available online as we reach this significant anniversary. In addition, I would be delighted to receive electronic copies of any photographs, old meeting programmes or historical correspondence for archiving and sharing *via* the **crystallography.org.uk** website.

The New Year will also bring elections for the roles of Vice-president, Secretary, and one Ordinary Member of Council. Of these, **Anna Warren** has served two terms as Ordinary Member and so is not eligible for re-election. Please note that although the Nominating Committee assists in recruiting candidates to stand for these roles, nominations can also come directly from any two members with the consent of the candidate and we strongly encourage members to make use of this method of nomination. Such nominations should be communicated to the current Secretary (**secretary@crystallograpy.org.uk**) by September 30th.

Planning is at an advanced stage for the **BCA Spring Meeting 2022**, under the careful watch of Programme Chair **Iain Oswald**. Just over a month ago I sat in on the first meeting of the programme committee and was excited to see another fantastic programme forming before my eyes from a thoughtful discussion of a wide range of competing ideas. Thanks to everyone who contributed ideas – especially the group representatives. The dates to block out in your diary are Monday 11th April until Thursday 14th April 2022 and the venue will be the University of Leeds. Further programme highlights are available elsewhere in this issue. I would also strongly encourage you to start thinking about contributing oral or poster abstracts to one of the scientific sessions – the abstract deadline early in the New Year always seems to arrive sooner than expected. Next year, as usual, the first afternoon and morning of the Spring Meeting will be organised and run by the Young Crystallographers Group. The speakers and poster presenters at these sessions are mainly students and early career researchers, but everyone is welcome to attend.

The BCA Prize Lecture is usually awarded triennially, with a small dislocation due to pandemic-postponed meetings, to someone who has made a notable contribution to scientific research in which crystallography has played a central role. The next lecture will next be delivered at the 2023 Spring Meeting and although this seems a long way in the future, we need to confirm invitations during the meeting planning process, so please send in a nomination as soon as possible and definitely before April. Nominations are welcomed from any part of the crystallographic community and should be sent by email to the BCA President (**president@crystallography.org.uk**) together with a short case supporting the nomination. I will confirm receipt – please double check if you don't hear back.

Thanks to *Crystallography News* editor **John Finney** for calmly and efficiently overseeing the assembly of this issue. John has another 6 issues to go before he comes to the end of his term, and while this still seems a while away, it's never too early to line up a smooth handover. If you have a passion for editing and communicating and would like to volunteer for this role, then please don't hesitate to get in touch with either of us to find out what is involved.

A reminder that the latest breaking BCA news can always be found on the @britcryst twitter feed. If you're not a twitter user then the latest posts can be seen on the front page of the BCA website **crystallography.org.uk** underneath the list of our corporate sponsors in the left-hand column. The twitter account can be used to keep an eye on meeting announcements, reminders of abstract deadlines and news from BCA members.

Finally, news of a special journal issue that may be of interest. The BCA is established as an educational charity, and most of its meetings and activities are organised to encourage dissemination and discussion of new ideas and discoveries. Educational and outreach activities may be targeted for Ph.D. students, researchers, and school children. Crystallographers working with a wide range of techniques and different materials are often united by an interest in crystallographic education and teaching, and many of the fundamental concepts required to teach about crystal structures and the scattering of waves are the same across our community. Given the recent upheaval in teaching practices due to the global pandemic I would like to draw attention to a very timely call for papers on "Modern approaches and tools for teaching crystallography" in a special issue of Acta Cryst. Section E – **https://journals.iucr.org/e/services/specialissues.html**. The deadline for article submissions is June 2022.

Richard Cooper

BCA Council 2021

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website **www.crystallography.org.uk**

From the Editor

JOHN Desmond Bernal died 50 years ago on September 15th 1971. Recognising his fundamental inputs into not only the experimental and theoretical development of crystallography, but also its exploitation in diverse areas, it seemed appropriate to devote a significant part of this month's *Crystallography News* to his work and his ideas. Accordingly, you will find two articles by colleagues who worked with him in his later years, and one by another colleague who joined the Birkbeck protein crystallography team soon after his death. Finally, we have an article that describes a new research institute in his home country of Ireland that was inspired by his commitment to the use of science for the benefit of society. I hope you enjoy these explorations of his fundamental crystallographic contributions.

The articles included here do, however, address only a part of his wide-ranging interests and accomplishments. It's not without justification that many consider him one of the great polymaths of the 20th century, though **Alan Mackay** (Birkbeck), who worked with Bernal for twenty years longer than I did, used the word 'polytropic' to characterise his being active in many dimensions and directions[1]. In addition to his 'classical' crystallographic work on small and large biological molecules, materials and liquids, he argued that 'classical' crystallography was only a limited part of what he termed 'Generalised Crystallography', a concept which was taken forward by **Alan Mackay**, who predicted the existence of quasicrystals and realised the three-dimensional version of Penrose tiling. Anyone interested in following up these ideas will find elements of them in Bernal's opening remarks to a CIBA symposium in 1966 on the Principles of Biomolecular Organization[2] and a fuller setting out of them in an article in *Kristallografia*[3] (I have copies of both these articles). He also saw very early on the potential of computing for crystallography in particular, so much so that one of the groups he insisted on including in the Biomolecular Research Centre he set up at Birkbeck in the 1940s was focussed on computer development.

Finally, it would be amiss of me not to mention at least some of his non-structural work. During the Second World War, he was a founding father and leading exponent of operational research, and as scientific adviser to Mountbatten, the Chief of Combined Operations, contributed a great deal to the war effort. A particularly interesting example that is often quoted relates to his detailed mapping and tidal conditions of the Normandy landing beaches. In fact, **Major Logan Scott-Bowden**, who was chosen to reconnoitre the proposed positions of the Mulberry harbours (huge concrete caissons with a flexible steel roadway laid over their tops), commented that "Bernal was crucial to the planning of D-Day. He was in charge of it in a way." Not bad for someone who liked to jokingly remember that he "committed the frightful solecism of not knowing which was port and which side was starboard". For anyone interested in either Bernal's science or other aspects of his life, I cannot recommend strongly enough the biography written by **Andrew Brown**[4].

Turning to more recent matters, I have recently been very disappointed with the BBC's coverage towards the end of July of AlphaFold – the AI system that performed impressively in the latest CASP (Critical Assessment of Techniques for Protein Structure Prediction) meeting. **David Jones** (UCL) and **Janet Thornton** (EMBL-EBI) wrote on this in the March 2021 *Crystallography News*, commenting that "the most exciting thing about this achievement is that it isn't the end of anything, but is really the beginning of many new things…this will enable the field of structural biology to grow and contribute even more to our understanding of life at the molecular level". Towards the end of July, Deep Mind released the source code behind the latest version of AlphaFold, and a detailed description of how it was developed[5]. Moreover, they have made available in a database maintained by EMBL-EBI the predicted structures of most known proteins encoded by the human genome, as well as those of 20 other organisms, totalling some 350,000 predicted structures. Impressive indeed and full marks for openness! But what got me was the BBC press coverage. First, the Radio 4 programme 'Inside Science' gave the impression that Deep Mind had finally completely solved the protein folding problem. Secondly, on the Radio 4 Today programme a day or so later, it was presented as pretty well the greatest development biological science has seen. In neither programme was there any attempt to get across to the listener the limitations, some of which were clearly set out in the *Nature News* article published on 22nd July6. While, as **David Jones** has said there[6] that it is indeed "an amazing first step", **Venki Ramakrishnan** (LMB Cambridge) is reported[6] as saying biologists will want to continue benchmarking these predictions to experimental data to get a better handle on their reliability. To quote **Christine Orengo** (UCL) from that article[6]: "We need to be able to trust these data". So like the success of AlphaFold in the latest CASP meeting, this impressive data dump is a beginning, not an end.

This failure of the BBC to do 'due diligence' on the matter would have given the general listener the impression that we now know the structures of all the proteins in the human body and therefore will soon be able to cure all the diseases that relate to protein functioning. When this nirvana is not delivered, might it help to fuel public scepticism of science more generally?

A pity that the BBC coverage could not reflect the balanced view of the *Nature News* article.

Stepping down now from my soap box, we say goodbye this month to two crystallographic colleagues. **John Reid** focussed his work on diffuse scattering and the information that could be extracted from it, while **John Squire** was internationally renowned for his research on the structural basis of muscle contraction – and also edited *Crystallography News* from 1987 to 1995. We shall miss them both.

John Finney

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5. J. Jumper *et al. Nature* https://doi.org/10.1038/s41586-021-03819-2 (2021).
6. E. Callaway. *Nature News* 22 July 2021 https://www-nature-com.libproxy.ucl.ac.uk/articles/d41586-021-02025-4.

Puzzle Corner

THIS quarter's puzzle comes in two versions – a simpler and a more challenging one.

Simpler one: Show how the plane group p2mg can be illustrated using the (lower case) letters b, d, p and q.

A little more ambitious: Show how all the oblique and rectangular plane groups can be illustrated using the same four lower case letters.

Solution to June's puzzle: (Sandy Blake's bathroom wallpaper)

The cell is rectangular in shape (thanks to the needs of paper hangers) but not in symmetry, which is clearly p1. There is, however, a pseudo centring of material, so all reflections with h+k odd will be systematically weak. A fairly small shift (with artistic limitations) would give a vertical glide line to give plane group pg. Taking this as the b-axis, 0k reflections would would then be missing for k odd. Bigger shifts could give the centrosymmetric cell p2 or a p1 cell half the size.

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John Desmond Bernal: 1901 - 1971

THE 50th Anniversary of J.D. Bernal's death seems an appropriate occasion to look at his fundamental role in the development and exploitation of Crystallography. The following three articles explore his influence on structural biology, material science and our understanding of liquid structure (including water). The final article describes his recent scientific legacy in Ireland (the country of his birth), which is helping to realise his concern that Science should be used for the benefit of Society.

Bernal's early influence on Biomolecular structure, and on Protein Crystallography

Bernal had the satisfaction of determining the atomic structure of graphite in the early days of X-ray crystallography under the guidance of William H. Bragg while at the Davy-Faraday Laboratory at the Royal Institution in London (1923-27). Bernal was less enchanted with the tedium of indexing the diffraction spots, and so he devised ways of aiding the interpretation of single crystal rotation photographs by inventing Bernal charts. His first two papers published in 1924 and 1926 brought him early recognition as a leader in X-ray crystallography. However, recognising even then the potential of the technique, he wanted to extend the reach of X-ray structure analysis to the biological world. As both he and his colleague Bill Astbury wanted to tackle proteins, they divided the field between them, Astbury taking on the fibres, Bernal the soluble globular proteins.

In 1927 Bernal moved back to Cambridge as Lecturer in Structural Crystallography in the Department of Mineralogy next door to the Cavendish. In his quest to understand the biological world he took advantage of the proximity of the Biochemistry Laboratory, led by Frederick Gowland Hopkins, who considered that enzymatic activity was responsible for the biological activity of living cells. Although little was known of protein structure at the time, it was known that chemically they were chains of amino acids. In the summer of 1928 Bernal travelled around European laboratories to catch up on progress in protein research. He began work on amino acids and related compounds using crystals prepared by A. Leese in Biochemistry. Atomic resolution structures of these molecules was beyond reach at that time, but Bernal had shown from his Cambridge student days that he had the kind of geometric mind that could independently derive all 230 space groups (see Paul Barnes's article in this issue). He therefore embarked on optical and X-ray characterisation of the unit cells, to reveal likely models of the amino acids and how they packed together in the crystals. The final paragraph of the survey published in 1931, reads: "A detailed account of the crystallographic investigation with a discussion of its chemical implications will be published at a later date. In the meanwhile, in view of the difficulty of obtaining crystals of these compounds the author would be very grateful if anyone possessing such crystals of a magnitude of .01 mm or over would send a few mgms of them to him for examination".

In the early 1930s Solly Zuckerman and J.B.S. Haldane steered Bernal towards new crystals of the sex hormone oestrin. He was able to figure out from unit cell dimensions, symmetry and optical properties that all steroids were likely to have a similar structure, which was not in agreement with the ideas of the leading chemists of the day. Bernal's observations led to a rapid reappraisal of sterol chemistry. The sterol success boosted Bernal's reputation among chemists and filled his desk with samples. In 1932 an Oxford graduate Dorothy Crowfoot joined him as a Ph.D. student. He invited her to sort out his desk and she became his principal photographer of biological samples.

Protein Crystallography begins

The key experiment performed by Bernal in 1934 that started protein crystallography is described in *Nature*, with an opening sentence that reads like a diary entry: "Four weeks ago, Dr G. Millikan brought us some crystals of pepsin prepared by Dr Philpot in the laboratory of Professor The Svedberg, Uppsala." On exposure to air the crystal birefringence diminished and X-ray photographs taken in the usual way showed nothing but a vague blackening. So Bernal drew a new pepsin crystal into a fine glass tube, surrounded by its mother liquor. To his delight this time there was a pattern of spots extending all over the film that sent him wandering the streets of Cambridge through the night. From the intensity of the spots near the centre, he proposed that protein molecules are relatively dense globular bodies, separated by relatively large spaces which contain water. From the intensity of the more distant spots, he inferred that the arrangement of atoms inside the protein molecule is of a perfectly definite kind, although without the periodicities

***Figure 1:** Dorothy Hodgkin discussing things with **Bernal**. Courtesy S. Jane Bernal.*

characterising the fibrous proteins, as determined by Astbury. Several more pepsin photographs were taken by Dorothy, but further interpretation was abandoned. The molecular basis of the activity of the enzyme pepsin was within grasp, but not yet.

Although Dorothy was not in Cambridge the day the first photo was taken, her name was on the publication. She remained in close contact with Bernal when she moved to Oxford later that year and acquired some insulin crystals. He mentored her through the X-ray work and pushed her to publish a single author paper in *Nature* in 1935 on her early results on dry insulin crystals. In 1935 in correspondence with Bernal on insulin she says: "It was clear that Bernal was thinking of the possibilities of changing zinc in the crystal for heavier metals and using the change to find the phase angles necessary for the direct calculation of an electron density map of insulin—the method of isomorphous replacement." Bernal's steering allowed her at a young age to be in a position to pursue independent research. Her subsequent application of X-ray crystallography to solve penicillin, vitamin B_{12} and insulin changed the way chemists approached the development of medical therapeutics.

Viruses. And Haemoglobin.

Isidore Fankuchen came to work with Bernal in 1935, ostensibly to work on sterols, having been trained in crystallography by W. Lawrence Bragg in Manchester. Instead Bernal had him work on plant virus particles, such as Tobacco Mosaic Virus (TMV), in collaboration with N.W. Pirie, who had purified a 'crystalline protein' from infected tobacco leaf sap. Bernal was keen to define the nature of the crystallinity. By measuring diffraction data from wet and dry gels and solutions, they showed the sample was in fact liquid crystalline. They deduced that the virus particles formed long rods that probably contained some RNA. Most of the diffraction peaks originated in the internal structure of each rod, for which Bernal, typically, had this to say: "A complete interpretation of this intramolecular pattern has not yet been possible; but a rough survey indicates that the molecule is made of piles of sub-molecules of dimensions 22 Å x 20 Å x 20 Å, somewhat smaller than the normal protein molecule, and themselves divided into nearly identical units with half these dimensions." But there was little interest in the substance, other than it was possible to follow the wake of a goldfish swimming in a solution of it when viewed under polarised light.

Bernal and Fankuchen were also intrigued by spherical viruses, and X-rayed crystals of Tomato Bushy Stunt Virus (TBSV). In Dorothy Hodgkin's Royal Society Biographical Memoir of Bernal, she tells us that: "The photograph was necessarily a powder photograph, though of wet crystals, and showed at first only two lines. With a pair of dividers and a ruler on the wet film, in great excitement, Bernal measured these lines and, assuming as was likely from the form of the crystal, that the lattice was cubic body centred, deduced a cubic unit cell of edge 390 Å, containing two particles of diameter 340 Å and a molecular mass of the order of 10 000 000." However, the more reflections they recorded, the less good the fit with any symmetrical model, so the work was paused.

When Max Perutz arrived in Bernal's lab. in 1936, he wanted to work on a biological molecule. With enthusiastic support from Bernal, he used his own initiative to get crystals of horse methaemoglobin, with the first diffraction photographs taken in late 1937. With help from Fankuchen, a Nature paper was rapidly published in March 1938. Wet crystals of both haemoglobin (and chymotrypsin) diffracted X-rays to high resolution with perfectly definite reflections at spacings as low as 2 Å, proving the internal regularity of the protein molecules down to atomic dimensions. Furthermore, controlled dehydration of the crystals caused variation in the intensities which Bernal saw may make possible the direct Fourier analysis of the molecular structure once complete sets of reflections became available in different states of hydration.

Birkbeck College

Bernal had ambitions to form an Institute of Biomolecular Research that would be organised at the boundaries of classical disciplines, but as he was disliked by the Head of the Cavendish, Ernest Rutherford, and out of favour with the University establishment, he could not progress his career in Cambridge. Early in 1938 Bernal was appointed Professor of Physics at Birkbeck College, University of London, taking over from Patrick Blackett. Formerly the London Mechanics' Institution, Birkbeck was organised so that working people could study for degrees in the evening, and so was more aligned with Bernal's politics.

The department was housed in the ancient Bream's Buildings, close to Chancery Lane. W.L. Bragg moved to Cambridge in 1938, having been appointed Cavendish Professor in succession to Rutherford who had died unexpectedly. Bragg and Bernal shared out the Cambridge apparatus and students. Max Perutz wished to stay in Cambridge with his crystals and Bragg was keen to keep him. Fankuchen went with Bernal to Birkbeck with the virus projects, soon to be joined by Harry Carlisle, a student from Burma.

Bernal summarised his thinking on proteins at a Friday evening discourse at the Royal Institution in January 1939, which was published the following April in *Nature*. He proclaimed that the phase problem can only be resolved by some physical artifice, such as the introduction of a heavy atom, or the observation of intensity changes on dehydration. The paper also includes his thoughts on "how the behaviour of the hydrophobe groups of the protein must be such as to hold it together … a force of association is provided which is not so much that of attraction between hydrophobe groups, which is always weak, but that of repulsion of the groups out of the water medium". Charles Tanford judges this overview as "a pioneering and prophetic paper, a glimpse into a rare moment when one man's insight was able to encompass simultaneously all the strands of a complex problem, much of which the rest of the protein community would not understand for another twenty years".

What Bernal – or anyone else – did not foresee at the time, was that a polypeptide chain could form a regular helix with a non-integral number of amino acids per turn. In the early 1950s Linus Pauling proposed the alpha helix which respected the planarity of the peptide bond, had around 3.7 amino acid residues per turn, with a predicted distance repeat of 5.4 Å, close to, but not exactly matching, the 5.15 Å repeat measured by Astbury in unstretched keratins.

In the summer of 1939 Bernal undertook an extensive trip to the U.S., visiting labs and giving lectures, including to the Rockefeller Institute. He made contact with Moses Kunitz, who specialised in crystallising enzymes, and this may have been the occasion at which he gave Bernal a tube of ribonuclease crystals. Bernal cut short the trip to return to the U.K. as war was coming. He evacuated his students and equipment to Dorothy in Oxford. (Harry Carlisle took his aging cholesteryl iodide crystals to her lab. and she guided him through the calculation of a 3D map phased from the heavy atom. The structure, announced in Cambridge in 1943, was the first time

a complex, asymmetrical biological molecule was visualised directly by X-ray analysis and opened a new way to determining unknown chemical structures). Bernal feared that outbreak of war would stop all work on proteins in Europe, so he dispatched Fankuchen to the U.S. with most of his materials in the hope he could continue there. At the start of the London Blitz, Fankuchen submitted a paper (from MIT, Cambridge) on X-ray diffraction of dry crystals of ribonuclease, while in the early hours of 25 September 1940 Birkbeck College was hit by incendiary bombs.

The War Interlude

In 1939 Bernal suspended his direct academic activities. He joined the Civil Defence Research Group, and in spite of his MI5 dossier, was recruited by a member of Chamberlain's cabinet, Sir John Anderson, who is quoted as saying "even if he is as red as the flames in hell, I want him". In 1942 Bernal became Scientific Adviser to Combined Operations under Lord Louis Mountbatten.

As an Austrian, Perutz became a refugee in 1938. He was arrested in Cambridge as an enemy alien in May 1940 and transported under appalling conditions to Canada where he was interned in a camp. He was able to return to his red crystals in Cambridge at the start of 1941, but was desperate to join the war effort. Bernal recruited him onto the doomed Habbakuk floating ice strip project (see Paul Barnes's article in this issue), based under Smithfield Market, a role which required Perutz to travel to the U.S. for demonstrations. The Home Office was pressed in 1943 to grant Perutz naturalisation, issuing him a British Passport with a U.S. visa. Max was soon able to network with U.S. protein scientists like John Edsall at Harvard and Martin Buerger at MIT, and to showcase his successful haemoglobin work. Meanwhile Bernal told Pauling he had "left the field myself for the duration and spend my time being an engineer, architect and explosives expert". However, Bernal went on to make more charts, this time for the landing beaches of Normandy. After D-Day, Bernal was sent to Ceylon. While testing bombs for jungle use alongside Wing Commander John Kendrew, he convinced Kendrew of the central importance of protein structure to understand the biology of living systems and directed him to Perutz in Cambridge.

The 'new' lab in a (very) old building

In 1947 the MRC agreed to support Perutz, Kendrew and a small team in a Unit within the Cavendish for five years.

Figure 2: *The Birkbeck Laboratory from 1948 to 1966.*

Francis Crick joined in 1949. Meanwhile Bernal's group was dispersed in temporary accommodation until his Biomolecular Research Laboratory, at 21-22 Torrington Square, was opened in July 1948 by W.L. Bragg. The research strategy was to exploit and enhance physical methods to understand the structure and function of soluble proteins and viruses, as well as to pursue research into materials and liquids (see articles by Paul Barnes and John Finney in this issue), in conjunction with development of computing methods. Bernal was looking for a link between long range interactions of proteins and biological systems, though was pessimistic about being able to buy the newly invented electron microscope. All this was expected to take place in a pair of partially repaired bomb-damaged Georgian houses in Bloomsbury that was supposedly temporary, but lasted for 20 years.

Although Bernal, like most scientists in the early 1940s, considered genes might be proteins, he recognised that chromosomes and viruses share a similar chemical composition. In his post-war Birkbeck lab., he directed Harry Carlisle to supervise Ph.D. student, Sven Furberg, who solved the structure of a nucleoside, cytidine. The puckered pentose ring was perpendicular to the flat base ring, an observation noted by Watson and Crick in their DNA double helix paper.

Getting a crystalline biological sample from an outside laboratory inside a well-equipped X-ray lab. and into the hands of a brilliant investigator was the recipe for advancement in the early days of biological structure analysis. In 1953 Bernal invited Rosalind Franklin to bring her fellowship to Birkbeck to follow up his pre-war studies of the rod-shaped TMV. Her X-ray diffraction photographs of oriented gels of TMV, which showed evidence of helical diffraction, enticed Aaron Klug to join her team in early 1954. They established the helical symmetry of TMV, showing it had 49 subunits per three turns of the helix. In 1955 Don Caspar, an American biophysicist on a fellowship in MRC Cambridge, came to work in Franklin's lab. They showed from a comparison of X-ray fibre diagrams of oriented gels of intact TMV virus and the reassembled isolated protein labelled with heavy atoms that the RNA was inside the helical protein shell, embedded in the protein subunits. Shortly before her early death in 1958, Franklin began work on poliomyelitis virus, sourced from Wendell Stanley, Berkeley. Klug and Caspar continued the polio work and raided the fridge for Bernal's old samples of spherical viruses. Caspar took the TBSV crystals while Klug and John Finch worked on the Turnip Yellow Mosaic Virus (TYMV). All turned out to have icosahedral symmetry, with 180 subunits. Caspar and Klug wrote their classic paper in 1962 on quasi-equivalence, taking inspiration from Buckminster-Fuller's construction of geodesic domes. This paper brought new ways of thinking about loosening regularity in modular protein assemblies, as well as a basis for the interpretation of virus electron micrographs. In 1962 Klug with John Finch and Ken Holmes, who had both gained their Ph.Ds at Birkbeck in 1959, moved to the newly opened MRC Laboratory of Molecular Biology (LMB) in Cambridge.

The phase problem was solved by Perutz in 1953, not by dehydrating crystals, but by introducing the physical artifice of a heavy atom derivative into haemoglobin enabling him to calculate the first two-dimensional electron density projection of haemoglobin. Kendrew was the first in 1960 to calculate a high resolution tertiary structure of a protein, monomeric myoglobin, showing rather unexpectedly that the alpha helices were not lying in an orderly parallel fashion. Perutz's team calculated the quaternary tetrameric structure of haemoglobin in 1968.

In 1950 David Harker accepted the challenge of building a

Bernal, Booth and the Double Helix

During the Birkbeck 2004 degree ceremony, Andrew Booth, a Bernal protégée, and a founder of Computer Science, whose multiplication algorithm sits in many contemporary laptops, was being made an honorary fellow. In his acceptance speech, Booth reported a story involving himself, Bernal, Rosalind Franklin and the Nobel Laureates Crick and Watson.

When Rosalind Franklin was at King's College before she moved to Birkbeck, Bernal arranged a meeting of these five to discuss the state of knowledge of the structure of DNA. The meeting was friendly and relaxed, and the participants were fully aware of the possibility of DNA assuming a double helix shape, since this was openly discussed at the meeting. Crick and Watson published their DNA double helix theory shortly afterwards. If this account is true, and I have no reason to think it is not, it may not rewrite history, but it adds to our knowledge of the timeline that led to the double helix discovery.

Paul Barnes

team to solve a protein structure for 1 million dollars. The Protein Structure Project was set up at the Polytechnic Institute in Brooklyn, following successful lobbying by Fankuchen, with ribonuclease as its target. A 2 Å structure was published in *Nature* in 1967. Without the luxury of such a large budget, Bernal and Carlisle started work on ribonuclease in the post-war years, trudging the painful path of searching for heavy atom derivatives. The structure was published in 1974.

Bernal had a mission to establish Crystallography as a distinct branch of science. In 1951 he began his difficult campaign with Birkbeck to extricate Crystallography from Physics into a separate department. In 1963 Bernal got his Chair in Crystallography, but the splitting of the two departments was delayed until 1967. Bernal's first stroke, which he largely recovered from, was in summer 1963. In late summer 1965 he suffered a disabling stroke, but his brain remained highly active, and he could, though with difficulty, communicate with colleagues, give lectures and write papers and books. He retired in 1966, just as the new crystallography laboratories were opened, and Harry Carlisle took the Chair. A couple of years later, Bernal had a heart attack and suffered a further stroke that left him essentially speechless for two years until his death on 15th Sept 1971. Carlisle continued protein research on ribonuclease, and new projects on plasma transferrins and eye lens crystallins were begun. Protein crystallography underwent rapid expansion when Tom Blundell, a former colleague of Dorothy Hodgkin, joined the department in 1976, taking the Bernal Chair in 1978.

Concluding comments

Bernal was clearly a – if not the – major driving force in the genesis and early development of biomolecular crystallography. The work he himself did in the 1920s and 1930s laid much of the foundations that have been built on by others. And his legacy can also be seen through the achievements of those he collaborated with and inspired – an impressive list that includes Caspar, Fankuchen, Finch, Franklin, Hodgkin, Holmes, Kendrew, Klug and Perutz. You can count the Nobel Prizes yourself.

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Bernal, Material Science, and Problem Solving

I first met Sage, as Bernal had been known since his undergraduate days, in his house, in 1968, after joining his Liquids Group as a postdoc. researcher. There is a record of that first meeting in Andrew Brown's biography[1], a book I recommend to anyone interested in Bernal. Though my meetings with Bernal were, due to his deteriorating health, intermittent over the three remaining years of his life, I drew inspiration from them and felt that I had touched greatness.

In my opinion he was one of the most powerful scientific thinkers of the 20th century, an intellectual giant within the vast field of structural science. He possessed a natural curiosity, endless enthusiasm, prodigious knowledge and brilliance with which he could explore the more remote regions of a subject outside the conventional boundaries of science. These are lofty claims so if any reader suspects exaggeration, a quick glance at the informed comments of eight Nobel Laureates (see box 1 on page 10) should surely set the record straight.

In this article, I take a quick look at some relevant events during his formative years, his search for research positions that complemented his skills and the turning points in his development. I am intrigued to see whether we can learn anything new from his choice of research projects or the open manner in which he carried them out.

The early days

While the boy Bernal showed clear signs of exceptional promise, his stellar potential only became fully recognised

Box 1: Comments on Bernal by eight Nobel Laureates (from reference 1)

Aaron Klug *(1982)*	"...was one of the most influential scientists of the 20th century."
James Watson *(1982)*	"...the extraordinary Irishman whose genius inspired the birth of molecular biology."
Francis Crick *(1982)*	"I regarded Bernal as a genius."
Linus Pauling *(1954)*	"... one of the greatest intellectuals of the 20th century."
Dorothy Hodgkin *(1964)*	"His greatest gift was his power to inspire others."
Hermann Muller *(1946)*	"One of the best, if not the best scientific mind in the world."
Lawrence Bragg *(1915)*	"He has been the pioneer who pushed the frontier forward."
John Kendrew *(1962)*	"It seems to me you've fathered 5 Nobel Prizes this year alone."

during his first year at Emmanuel College, Cambridge. There he would be able to sample the full Cambridge educational package comprising not only the necessary science components but also the essentials of a fully rounded academic life with activities such as political discussion, debating, networking and meeting influential thinkers. Bernal thrived in such an environment which in turn brought out the very best in him, accelerating his transition towards the later accomplished version that we would eventually recognize.

Bernal enjoyed listening to lectures that explored the dimensionality of a given topic and was clearly developing a flair for solving geometrical problems. In 1921 he set himself the challenging project of deriving the 230 Crystallographic Space Groups using the Quaternion mathematical representation. His wife to be, Eileen Sprague, assisted by typing the 80-page document which was then shortened to a 60-page version full of densely packed mathematics with no diagrams. It won him a shared first prize of £30 from Emmanuel College but the effort and time that he devoted to it may have cost him the first class honours he wanted so badly.

Bernal's next task was to find a post that fitted in with his areas of expertise in crystallography and that could provide him with a salary. The Cavendish could not help him. However, he did succeed in getting some temporary support from his old college, Emmanuel, which kept him and Eileen alive until he was able to join W.H. Bragg at the Royal Institution (RI).

Bernal at the Royal Institution

Bernal's stay at the RI from 1923 to 1927 comes across as a happy period in spite of a clumsy start. The laboratory exuded a friendly informal atmosphere which encouraged cooperation. In addition, Bernal and Eileen melded effortlessly into the London social and political scene which in turn was well-suited to the Bernals' unconventional lifestyle. Bernal started slowly in the lab., but then excelled himself by making significant improvements to the X-ray equipment and production of crystallographic manuals and charts and teaching aids. However, these endeavours were all over-shadowed by one single Bernal breakthrough, the determination of the structure of graphite. This was hugely significant for several reasons:

- Several big names in crystallography had tried to solve its structure, but all had failed. Bernal, however, demonstrated he had the patience to succeed and even constructed a home-made X-ray diffraction camera from various discarded objects (brass tubing, bicycle clips, alarm clock, bent nail – see figure 1). Needless to say, he had to perform all his calculations by hand!
- There was a long-standing paradox regarding diamond and graphite. Both are made from carbon alone, yet diamond was the hardest material known to man while graphite is a very soft material. Bernal's explanation resolved the paradox on the basis of the differences in structure: diamond has strong covalent bonds in a tetrahedral arrangement, thereby imparting strong interactions in all directions, whereas the graphite structure consists of hexagonal layers that can slide over each other like cards in a deck, resulting in softness and a tendency to smear. Obvious now to us as we accept that properties are related to structure (hence Crystallography!), but not realised before Bernal explained it.

Figure 1: *Bernal's prototype rotation camera!*

Following his four years at the RI, Bernal held a lectureship in Mineralogy and Crystallography at Cambridge until he moved to Birkbeck College in 1938, where he was to remain until his death.

Bernal, Birkbeck and World War II

With the likelihood of war against Hitler's Germany, Bernal felt compelled to voice his protest at the lack of preparation for mounting any form of response against an initial attack. He and Solly Zuckerman, a medic turned bio-scientist and anthropologist, became an effective duo in challenging the politicians' official lines. Perhaps in line with U.S. President Lyndon Johnson's infamous remark about preferring his antagonists to be inside rather than outside his tent, Lord Louis Mountbatten in April 1942 invited Bernal to become his scientific advisor in Combined Operations. Bernal accepted and set about designing arrangements that would enable him to work on Combined Operations while remaining in contact with Birkbeck and Crystallography via some kind of partial leave of absence. The complex arrangements, formal and informal, considerable deputising, delegation and shuffling of duties eventually brought about a successful arrangement, but not without heavy negotiations and quite a few headaches.

Bernal's scientific interests were extremely broad, both with respect to science itself and the use to which science could be put. His Birkbeck department reflected this broad range, with research groups focussing on Structures of Biological Systems[2], Materials Science Structures (initially headed by Helen Megaw, and which I took over following the retirement of Jim Jeffery), Structures of Liquids[3] (the Group which I originally joined) and Generalised Crystallography (in which Alan Mackay was a major collaborator).

This eclecticism is reflected in not only the strictly structural problems of, for example, graphite, bronze, metals and alloys, proteins, viruses and liquids, but also in the application of scientific methodology to 'real' issues exampled by many of the problems he was concerned with during the war – see box 2.

Box 2:
Some war-related projects of Bernal's

- Efficacy of gas masks with respect to poisonous gases
- Action of incendiary bombs on building top floors
- Design of effective shelters
- Blast management
- Physics of explosions
- Biological effects of explosions
- Resistance of concrete and other materials to explosions
- Handling of unexploded bombs (Bernal risked his life many times by defusing real unexploded bombs)
- Physics of air raids
- Statistical analysis of bombing raids
- Effects of breakwaters in sinking boats
- Properties of Pykrete
- A synthetic Iceberg as an airstrip for bomber operations

While much of what Bernal accomplished wasn't crystallographic – even within his wide interpretation of the subject – I give below an example of his non-crystallographic war work, followed by one war project which certainly did relate to materials and their functionality. Finally I say something about the work that involved me – the polywater story.

(a) Statistical analysis of bombing raids

If there was one science area above all others in which Bernal, as scientific advisor, had left his distinctive mark it would, I believe, be on his use of statistical analysis; one might call it Bernal's war-time legacy. Bernal took its implementation to a new level, in terms of both the surveying and the interpretation of the raw data. This was particularly so for assessing the effectiveness of bombing raids of both sides in causing both physical and psychological damage.

An assortment of volunteers and students, as well as professional statisticians, were used to establish relationships between damage, tonnage of bombs deployed, type of environment ascertained from observation, previous conflicts, and accurate maps. Similar methodology was used to measure loss of morale using medicinal changes and increased alcohol consumption as indicators of population morale. Interestingly, the loss of morale in the affected population was generally less than expected. The rigour and neutrality behind the data from the statisticians were as a breath of fresh air compared to the unverified and sometimes exaggerated claims made by those carrying out the 'work', such as flight crews. One issue of great irritation to the statisticians was the ignoring of their predictions, meaning the lives of pilots were sometimes being put in danger unnecessarily as they carried out bombing missions that statisticians had already shown to be of little value.

I close this section with an anti-intuitive statistical gem: more damage was inflicted on RAF aircraft parked on the ground than during aerial combat.

(b) Habakkuk

Habakkuk was an old Testament Prophet who invited the heathen to look upon his unbelievable works in fear ("I will work a work in your days which ye will not believe, though it be told you")[4]. So, it was perhaps appropriate that Habakkuk was used as the name for one of the most imaginative and ambitious projects of World War II: to produce man-made icebergs to serve as gigantic aircraft carriers. The reasons for Habakkuk were not obvious, nor was it obviously feasible. However, consider the following remarkable attributes.

- The cost of the building materials is virtually zero;
- The breakup cost is virtually zero since the main component simply melts away;
- The project is ecologically 'green';
- The project is economically independent of how long the structure operates;
- The structure is mobile with a range of thousands of miles, and so can be positioned to match war requirements;
- The structure would need to last for only a few years, unlike a commercial equivalent.

With these points taken into account the project does appear attractive. The iceberg would be powered by a number of propelling units, and steered by a combination of those units and a gigantic rudder. Inside the structure would be refrigerator units supplementing the natural environmental chill, keeping it at sub-zero temperatures. To give some idea of the feasibility of staying cool, a scaled-down model was built that took two years to melt naturally.

The icebergs were to be built using pykrete – a mixture of 15% wood shavings and 85% ice. This material, named after its inventor Geoffrey Pyke, has remarkable strength, and melts very slowly. The plan was to make each of these icebergs the size of 25 aircraft carriers.

If correctly constructed, pykrete blocks are stronger than concrete by weight and their thermal conductivity is lower than ordinary ice by an order of magnitude – the wood shavings behave as thermo-mechanical barriers. It was what we now know as a composite material; then, it was 40 years ahead of its time.

It was a controversial project. Some believed it was outlandish. Others including Churchill thought it had sufficient merits to be worth a try. The pykrete block was tested by Max Perutz[2] – the same Perutz who went on to win with John Kendrew the Nobel Prize for his work on haemoglobin.

A somewhat amusing scene took place in a briefing session on board the Queen Mary (see figure 2 below).

A block of pykrete and a block of ordinary ice were presented to an audience, which we believe included Churchill. One General Arnold attempted to break the ice block with an axe. He succeeded easily. When trying to break the pykrete block, not only did the axe fail to cause any damage, but also the resulting shock-wave travelling up Arnold's arm caused him to gasp in pain.

In typical dramatic style, Mountbatten decided to repeat the experiment, but with a revolver. The ordinary ice shattered. In contrast, the pykrete block suffered little damage. Moreover, the bullet ricocheted off, narrowly missing one of the observing officers. It is said that pykrete was demonstrated by Churchill at dinner parties. He would present two apparently similar blocks of ice, but one of them would appear not to melt, or would melt only very slowly, presumably amazing his guests.

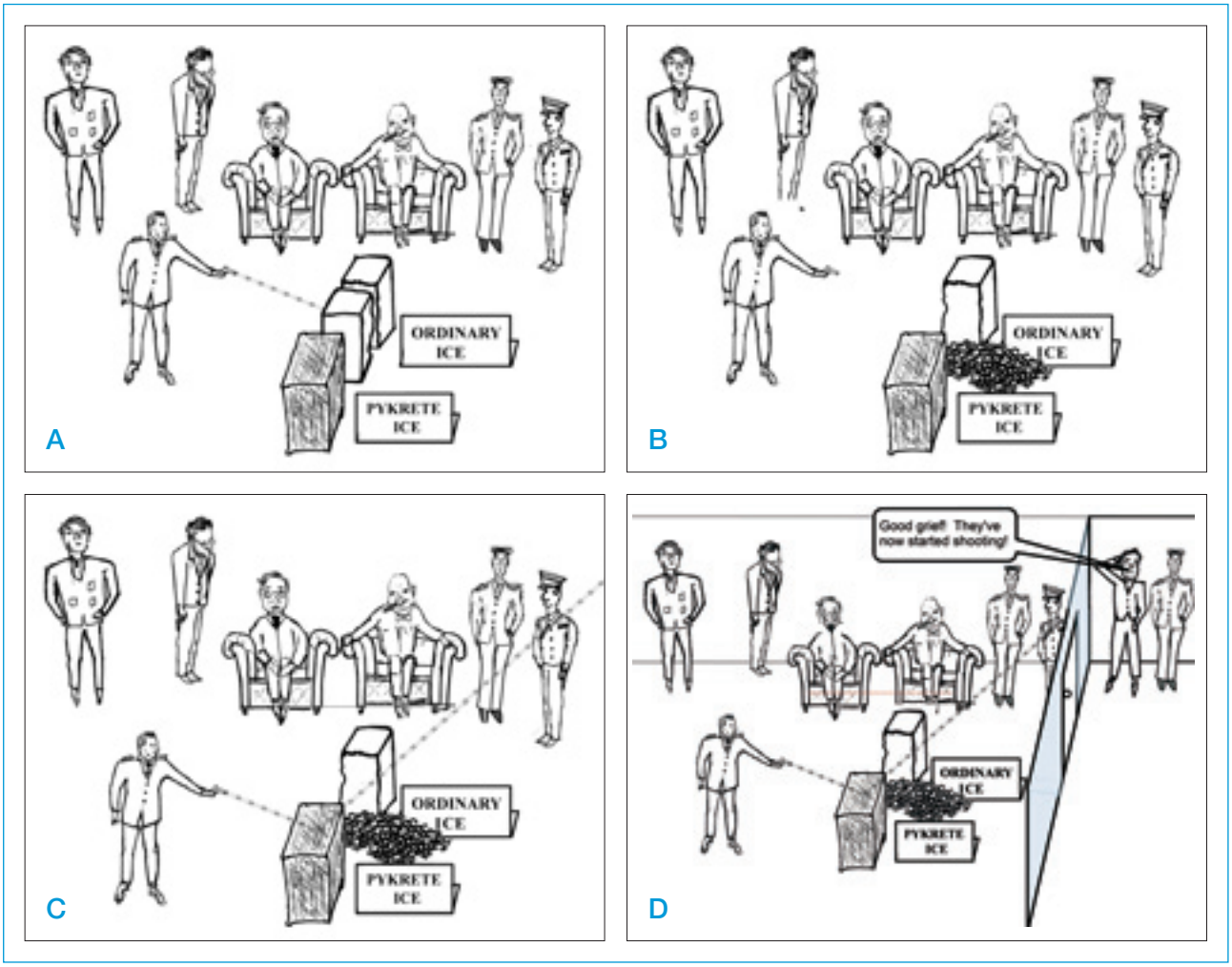
Despite these positives, the project was turned down after the requirements expanded. The required travelling range grew to 7,000 miles, the required lifetime expanded to 3 - 5 years, and the weight to be carried grew from that of fighter planes only to bombers and fighters. These increases in requirements, and the increase in distances that aircraft could fly without refuelling, combined to result in the project's cancellation.

(c) Polywater

Polywater was the name given to an allegedly new structural form of water being worked on by the Russian group of Boris Deryaguin, and was being followed up by various international groups. I was aware of the work of Deryaguin mainly because of his classic publication on the DLVO theory of surface interactions. He had a high reputation in the scientific world, so when he made the surprising claims regarding the existence of a new from of water, he was given the benefit of the doubt. He claimed that water could be persuaded to condense onto confined silicate surfaces (e.g. glass or quartz capillaries) in a form that exhibited significant changes in its physical properties, such as boiling point, freezing point, and density-temperature profile. Deryaguin's claims went further: he said that when ordinary and polywater droplets co-existed in proximity but with no physical contact, the polywater droplets could grow at the expense of the 'ordinary' water droplets. He was saying ordinary water could transform easily into polywater, implying polywater was a more stable form of H_2O.

When I was a post doc. researcher in Cambridge in 1968, I attended a lecture on polywater given by Deryaguin who was

Figure 2: *The pykrete test!*



visiting the UK. I then wrote to Bernal at Birkbeck and asked if I could join his team which I had heard was to start research into polywater. Thus my four decade career at Birkbeck began. So in some ways Deryaguin was responsible for my association with Birkbeck. This is somewhat ironic, since he later tried to get me – and the rest of the team (including the current editor of *Crystallography News*) – sacked.

At the time I joined Birkbeck, the scientific community was full of polywater rumours and counter-rumours, and these extended into the wider academic world, industry and government. The issue started to feature in mainstream newspapers and TV. I was even interviewed about polywater, along with some of my Birkbeck colleagues, by the BBC.

Several *ad hoc* scientific meetings were arranged to address the issue. I remember one in particular in 1969, attended by about 40 physicists and chemists. The morning session consisted of everyone having an opportunity to describe their experiences making or using the alleged polywater. Reports fell into three categories:

1) I am trying hard but cannot make any polywater.
2) I can make polywater, and I am trying to measure some property (e.g. X-ray spectra, boiling point, freezing point).
3) Beware of the misleading effects of surface chemistry.

At the end of that meeting, various follow-up meetings were arranged to take place depending on the outcomes of further work. It may be that none ever took place...

Further communications on the subject became progressively quieter and less frequent when the Birkbeck group decided it was time we went public with the results of our work on the problem: that all such 'sightings' were nothing more than surface effects and contamination. And there was no real danger to our planet, as there would have been had 'polywater' indeed been a more stable form of H_2O as claimed by some polywater adherents. We said polywater did not exist; what others had found were just 'polypollutants'[5].

After publication we waited for the response which we expected would be an onslaught of invective against anything found carrying the name of Birkbeck. In the event it was the opposite: near-silence except for a letter from Deryaguin to Bernal urging that the Birkbeck team should be sacked for incompetence! Communications on polywater then appeared to vanish altogether, its champions seeming to have given up and moved onto other projects. Polywater was dead, killed by a deafening silence.

I think Deryaguin had been reporting what he believed to be true, based on information given to him by his experimental colleagues. He himself was more of a theoretician. A few years after our paper, Deryaguin, to his credit, retracted his previous claims in print.

A final comment

A question about Bernal: one long mission or multiple short-term solutions?

While waiting for a bus I sometimes play my mind game *Categorize* in which I try to place all members of a chosen group into the lowest possible number of categories. For example if the group comprised all famous crystallographers, dead or alive, known by me, I might try to sub-divide the members into two categories: those who are driven or inspired in their research as part of a life-long mission (e.g. seeking a cure for cancer; developing the theory of relativity) and those who are driven by the repeated thrill of solving many short-term problems (e.g. regularly solving the Times crossword). I can usually make an informed choice between the two but when the case of Bernal comes up, clarity disappears, as I uncover signs in his history that can apply to either of the two form of inspiration. This ambiguity might in turn be related to another of Bernal's renowned abilities, that of *multi-tasking*, evident long before the modern use of the term had been invented.

So the answer to the above question is that Bernal was in both categories.

Concluding remarks

In my opinion Bernal was one of the greats, both for who he was and for what he did. His abilities included an amazing memory, a fertile imagination, and a determination to work for the benefit of mankind.

I rate him as one of the four founding pillars of X-ray Crystallography. Röntgen discovered X-rays; von Laue confirmed X-ray diffraction; the Braggs used X-rays to reveal crystal structure. For me, the fourth pillar is Bernal, since he linked the above discoveries and systematised X-ray Crystallography.

A case could be made that Bernal should have been awarded whole or part of four Nobel prizes: a share in the one awarded to Dorothy Hodgkin, a share in the one awarded to Max Perutz, and two prizes, that were never awarded, for his founding work linking X-ray diffraction with structure, and properties and function of crystalline materials. As to why Bernal was never a Nobel laureate, the reasons offered range from political forces, to being active in too many different areas of science. These reasons are still debated now, 50 years after his death.

One final remark. Over the last 18 months we have seen scientists around the world work together for the benefit of mankind as they delivered vaccines effective against Covid-19. The level of cooperation and the speed with which life-saving results have been delivered has been unprecedented and remarkable. This is exactly the role that Bernal wanted for science. If he had lived to see this, he would have been very happy.

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Acknowledgements

This article is derived from my own experience plus a host of discussions and written sources too numerous to mention, with the exception of Andrew Brown's excellent biography[1], which has been my main written source. Special thanks are due to Michael O'Callaghan, friend and colleague, who has been a huge help in the research and writing of this article.

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Bernal, Water and Liquids

Though Bernal threw out ideas for others to develop, he kept the development of his approach to liquids for himself. Initially, his interest was sparked by the biological relevance of water, saying "My interest in the subject ...came about...through my biochemical interests, in that all living structures are mostly composed of water"[1]. This interest was to lead to a landmark paper in 1933 published in the first number of the Journal of Chemical Physics[2]. Bearing in mind that this was only 20 years since X-rays were first diffracted from a crystal, and barely a decade since the first methods of working back from a diffraction pattern to a crystal structure were successful, to tackle the much more difficult problem of liquids, where there was inadequate understanding of how to interpret the broad diffraction patterns that liquids gave, was ambitious to say the least.

Arguing that the charge distribution on a water molecule was near-tetrahedral, Bernal proposed that as opposite charges would attract, the local molecular structure should be essentially tetrahedral (see figure 1).

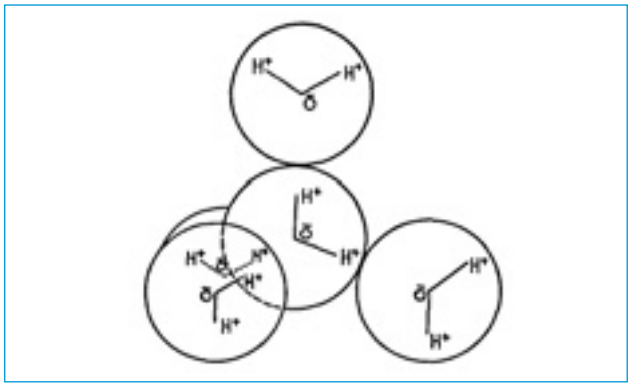
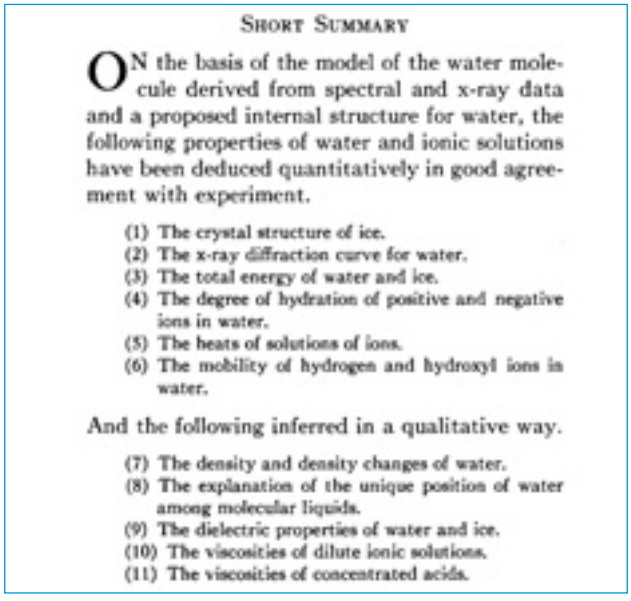


Figure 1: *The ideal local tetrahedral arrangement of water molecules as first envisaged by Bernal in 1933. Two of the four molecules surrounding the central one are in the plane of the paper, while one is above and one is below it.*

Noting that silica (SiO_2) also forms similar local structures, he developed 'disordered' versions of two silica structures (quartz and tridymite) to fit the X-ray data. With this model, he was able to explain a wide range of the properties of water and ionic solutions, as listed in the short summary heading that paper shown in Figure 2.



SHORT SUMMARY

ON the basis of the model of the water molecule derived from spectral and x-ray data and a proposed internal structure for water, the following properties of water and ionic solutions have been deduced quantitatively in good agreement with experiment.

(1) The crystal structure of ice.
(2) The x-ray diffraction curve for water.
(3) The total energy of water and ice.
(4) The degree of hydration of positive and negative ions in water.
(5) The heats of solutions of ions.
(6) The mobility of hydrogen and hydroxyl ions in water.

And the following inferred in a qualitative way.

(7) The density and density changes of water.
(8) The explanation of the unique position of water among molecular liquids.
(9) The dielectric properties of water and ice.
(10) The viscosities of dilute ionic solutions.
(11) The viscosities of concentrated acids.

Figure 2: *The 'Short summary' of Bernal's classic 1933 water paper.*

It is also worth noting that the not-quite tetrahedral charge distribution he used is essentially the father of the effective pair potentials used today in simulations of water and aqueous systems.

In Birkbeck, he returned to the water problem in the 1950s, when he recognised that his 1933 approach "was, frankly, one of crystal structure, trying to picture water structure as that of a mixture of the analogous four co-ordinated structures of … quartz and tridymite", and that "This was ultimately to prove rather a delusive approach, postulating a greater degree of order … in the liquid than actually exists there"[1].

However, rather than return to the specific problem of water, he recognised that he first needed to understand the structures of simpler liquids. Theoretical approaches to the liquid state at the time treated liquids either as disordered (crystalline) solids (as Bernal had done in the 1933 water paper) or as dense gases. Though the disordered crystal approach was mathematically tractable and could yield correct densities, it assigned too much order to the liquid – the predicted entropy was too low. On the other hand, treating liquids as dense gases required unphysical mathematical approximations: though the entropy could come out OK, the densities that could be handled were too low to be representative of real condensed phase liquids.

Bernal found both these approaches unsatisfactory. So instead he tried to find an approach that:

- was a concrete picture of the structure (Bernal was a crystallographer and so naturally would want to visualise the atomic arrangement);
- was consistent with Ockham's razor ('entities should not be multiplied beyond necessity');
- was homologous to that of the crystalline solid as well as radically different in kind;
- had a general quality of homogeneity without the assumption of any special groups.

The most general hypothesis he came up with was to treat the liquid "as *homogeneous, coherent* and *essentially irregular* assemblages of molecules containing no crystalline regions."[1] This concept he realised in the laboratory with assemblies of steel ball bearings, contrasting liquids as irregular *heaps* of molecules as against crystals as regular *piles*. Figure 3 illustrates the differences!

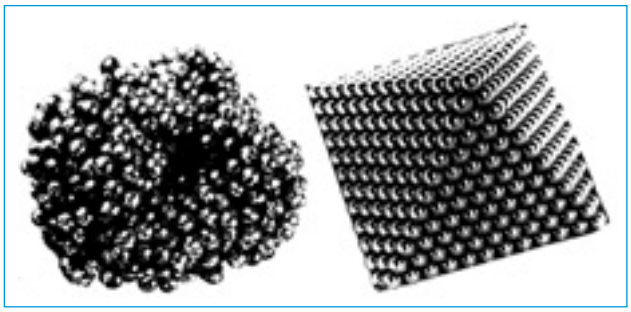


Figure 3: *Bernal's concept of the simple liquid as an irregular heap of molecules (left) compared to the regular pile of the crystal (right).*

This structural approach was indeed radically different from that of other workers on the liquid problem – and indeed Bernal apologised to "the modern theoretical physicist for introducing such a simple way of looking at things, but I believe on the whole that it is better to start with a model that has some resemblance to reality"[3].

And indeed the model was successful for simple liquids such as those of the inert gases. It gave correct densities, explained density changes on melting, had the right degree of disorder,

and essentially predicted the observed X-ray scattering. In the late 1960s, it was also successful in explaining structures of amorphous metal alloys. The coordinates of a large laboratory model on which much of the later work was based continues to be requested and used for a variety of theoretical and practical purposes[4]. And John Ziman, a key theoretician of liquids in the second half of the 20th century, commented that "This simple idea…is now seen to be the key to any qualitative or quantitative understanding of the physics of liquids"[5]. Similar comments were made in 1970 by John Rowlinson of Imperial College, one of the foremost theoretical chemists who has spent a lifetime working on liquids:

"It has therefore been hard to admit that the form or even the existence of the attractive forces has little direct effect on the structure of a liquid, as described, for example, by the pair distribution function g(r). The recent realization of this truth has followed the extensive studies … of the properties of assemblies of hard spheres without attractive forces."[6]

Recent work is also suggesting that Bernal's model can explain the behaviour of liquids above the critical point, where the liquid/vapour coexistence line that vanishes at the critical point continues into the supercritical region as a line of maximum heat capacity[7].

So how did Bernal move from this 'irregular heap' model to the more complex water problem? Simply by recognising that a disordered non-crystalline arrangement could also be built up of molecules interacting in the essentially tetrahedral fashion of figure 1 to produce a random *network* of molecules, as against the random *packing* of the spherical molecules of simple liquids. Figure 4 shows a ball and stick visualisation of a random network compared to the ordered crystalline arrangement of hexagonal ice.

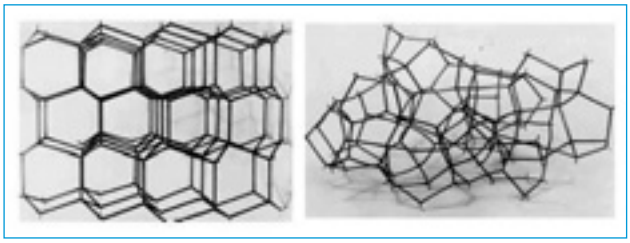


Figure 4: *A 'spaghetti model' visualisation of (left) crystalline ice Ih, compared with (right) the 'random network' arrangement of liquid water.*

So Bernal's final view of water[8] was that:

- Water is essentially a 'random network' of water molecules.
- Each molecule interacts with its neighbours in an approximately tetrahedral geometry.
- Local coordination is ideally 4-fold, but with some variation.

And it compared well with experimental results. It explains the main properties of water such as expansion on freezing, the temperature of maximum density and other so-called anomalies, the mobility of hydrogen, and structural changes with temperature and pressure. It is consistent with current state-of-the-art experimental and computational work, which demonstrates that Bernal's random network concept is essentially correct. And it has indeed helped us to understand water's biological role – the reason that Bernal started working on the problem in the first place.

John Finney
UCL

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Bernal's Irish connections and his enduring legacy at the Bernal Institute

John Desmond Bernal was born at the dawn of the 20th century (1901) and subsequently became one of the pioneering scientists associated with that century and the renaissance in science which it heralded. He addressed the big questions of his day. For instance: what is life and how did it originate[1]? He was convinced that the answer lay within the structure of matter and the molecules where form and function would be closely entangled. Those he inspired were subsequently involved in the nascence of structural biology (see article by Christine Slingsby in this issue) and were duly acknowledged for their pioneering work by the Nobel committee. It is fair to assert that Bernal laid the groundwork that ultimately led to the extinction of the 'vital force' postulate in much the same way that Einstein's relativity theories banished the luminiferous ether. Bernal was very much aware of the important role played by science in history, as is clear from his four volume book set of that title[2], and of its critical role in shaping society and so was active in pioneering the use of scientific methods to solve major social[3] and political[4] problems of his time. For a comprehensive account of his life and work, Andrew Brown's biography is a most interesting and engaging read[5].

Bernal was born in Nenagh, Co. Tipperary before Ireland won its independence. He was therefore a British citizen. Nevertheless, he was deeply 'imprinted' by his Irish childhood. He traced his roots to a mid-nineteenth century Sephardic Jewish migration. His grandfather, John Bernal, ran a successful auctioneering business in Limerick city and was also active in Limerick city politics. Around 1900, John Bernal's son, Samuel George Bernal (J.D. Bernal's father) bought a 147 acre country estate on the outskirts of Nenagh, complete with estate house, Brookwatson[6]. Considering those class conscious times, this is likely to have placed the Bernals amongst the Anglo Irish landed gentry ruling class. The 1911 Irish census lists those staying at Brookwatson to include his parents, siblings, two relatives and four servants[7].

Bernal Commemoration

Until recently, Bernal was largely unknown in Ireland although better established if neglected among our colleagues in the UK. In recent times, Bernal's contributions to science and to society have been acknowledged and he has been commemorated in various ways both in the U.K. and Ireland. On the occasion of

the unveiling of a plaque (on July 20, 2005) in honour of J.D. Bernal by the National Committee for Science and Engineering Commemorative Plaques in his home town of Nenagh (see Figure 1), Martin Bernal (J.D. Bernal's son) wrote: "Now, 35 years after his death, John Desmond Bernal has received this ultimate accolade". In 2006, the Munster branch of the Institute of Physics in Ireland organised a conference entitled 'John Desmond Bernal: Science and Society' with keynote speakers who knew and worked with Bernal[8,9]. Earlier, in 2001, An English Heritage blue plaque was erected at 44 Albert Street, London, where Bernal lived. And in 2013, after some years of planning, the magnificent Bernal Institute was opened by the Taoiseach (Irish Prime Minister), Mr Enda Kenny, on the University of Limerick riverside campus.

Figure 1: Pictured (photograph by V. Casey) in front of the science and engineering commemorative plaque to John Desmond Bernal are (L to R) ***Prof. Alan Mackay, Dr Martin Bernal, Prof. John Finney, Prof. Helena Sheahan*** *and* ***Dr Andrew Brown.***

The Bernal Institute, University of Limerick

In October 2010, the University of Limerick, arising out of ongoing work with Atlantic Philanthropies, prepared an ambitious Science and Engineering development plan under the stewardship of Professor Kieran Hodnett. Coinciding with the publication of Andrew Brown's book[5], the University of Limerick (UL) had an ideal opportunity to celebrate the life and achievements of a local lad (Nenagh lies just 35 km from the University of Limerick campus), who was one of the most influential scientists of the 20th Century. This was the genesis of the Bernal Project and preliminary planning for the Bernal Institute (BI) started in early 2011.

The Bernal Project ultimately resulted in a €100+ million investment in people and buildings to enable spatial integration of Science and Engineering disciplines at UL. The vision was to support synergies that result from close multidisciplinary collaborations and strong links with an Irish and international industrial base forged through UL's 'cooperative education' programme, an industry-academia education partnership. The overall project objective is to address societal challenges that require disruptive new technologies enabled by materials science and engineering.

The preliminary proposal envisaged the recruitment of ten Bernal Professors to act as international leaders in their fields and to develop the resources, equipment and infrastructure needed for the successful pursuit of both fundamental and applied research. Bernal was an extraordinarily generous mentor to younger colleagues. In appointing Bernal Professors UL therefore sought out candidates who would exhibit this same generous spirit of mentorship. A preliminary schedule of accommodation for the new building envisioned ten specialised laboratory suites in a 6,000m^2 building, with associated office and write-up space, seminar rooms, lecture theatres and social space. The total cost of the project was projected to be 52 M€. The BI project proposal was accepted for funding and an activity whirlwind of building design and recruitment followed with a three year timeline.

In September 2013, prior to the official launch of the Bernal project, the President of the University of Limerick hosted a dinner for some family members and friends of Professor Bernal. The attendees included Gay-Caroline Bernal (Bernal's granddaughter) who regaled the company with her childhood memories of visiting her grandfather in his offices in Birkbeck College, London and playing with his modelling materials including, we suspect, those used in models to support his theory of liquids (see article in this issue). Friends present included John Finney, UCL, a former external examiner to UL's applied physics degree and a previous student of Bernal's. Also present was R.J. Polle (Jack), just retired from active service as a vet having served the Brookwatson farm for over 70 years. He remembered meeting Bernal in 1950 when even at that stage, Bernal predicted how global warming caused by CO_2 emissions would lead to climate change.

By the time the Bernal Project was officially launched in October 2013 by 'An Taoiseach', seven of the ten Bernal Chairs had been filled (Figure 2) and the building aspect of the project was concluded in 2016 (Figure 3). Three additional chairs have subsequently been filled in composite materials, process engineering and structured materials.

Figure 2: Official launch of the Bernal Institute: (L to R) ***Prof. Edmond Magner****,* ***Prof. Don Barry*** *(President UL),* ***Prof. Bartek Glowacki*** *(Bernal Chair in Energy),* ***Prof. Gavin Walker*** *(Bernal Chair in Pharma Powder Engineering),* ***Prof. Ursel Bangert*** *(Bernal Chair in Microscopy and Imaging), An Taoiseach* ***Enda Kenny*** *TD,* ***Prof. Jacques Huyghe*** *(Bernal Chair),* ***Jon O'Halloran*** *(BI Operations Manager),* ***Prof. Michael Zaworotko*** *(Bernal Chair in Crystal Engineering),* ***Prof. Harry Van den Akker*** *(Bernal Chair in Fluid Mechanics),* ***Mary Shire*** *(Vice President Research, UL). Photograph courtesy UL.*

Figure 3: The sun about to rise over the Penrose tiling patterns that decorate 'The Cube', the large lecture hall in the Analog Devices Building of the Bernal Institute. Photograph courtesy M.J. Zaworotko.

Bernal's Enduring Science Legacy – The Bernal Institute

Bernal had many and varied interests, making key scientific contributions in his own time. He remains highly influential in many scientific domains. His early work on graphite[10] for instance has laid the foundation for the recent burgeoning research related to graphene[11]. For a comprehensive bibliography of Bernal's writings see Dorothy Hodgkin's Royal Society Biographical Memoir[12].

Some Ongoing Bernal Institute Projects

Under the umbrella of 'structures matter', the BI has developed five research clusters that span the full range of matter length scales and materials: (a) biomaterials; (b) molecular and nanomaterials; (c) 3D electron diffraction; (d) composite materials; (e) process engineering. Each of these clusters engages in research projects targeted at societal challenges related to sustainability and/or human health. The clusters are supported by world-class imaging facilities and molecular modelling research groups. Some highlights of the research in these clusters, several of which involve the study of crystals including crystal growth, are summarised below.

(a) Biomaterials

The Biomaterials Research Cluster focuses on structured biological materials, and systems based on molecular and cellular building blocks that range from molecular ensembles to cells/cell aggregates, tissues, and organs, and the interface with non-biological materials such as implants, drugs, and their combination. Prof. Tewfik Soulimane studies how diphenylalanine (FF) demonstrates a robust ability to self-assemble at the nanoscale forming a variety of structures ranging from nanospheres to nano- and microtubes resulting in outstanding functional properties including pyro- and piezoelectricity. FF nanotubes mimic the structure of β-amyloid fibrils characteristic of Alzheimer's disease and thus can serve as a model material in biology and medicine. Water confined in self-assembled FF peptides displays the properties of both bulk and nanoconfined water – confined water is critical to understanding the role of water in molecular biology where almost all water can be considered as confined water and/or mixed with ions and other molecules in aqueous solutions. Profs Tofail Syed and Damien Thompson study how piezoelectricity can be controlled through the self-assembly of amino acids. Piezoelectricity has attracted recent interest due to its manifestation in biological molecules such as synthetic polypeptides or amino acid crystals, including γ-glycine. It has also been demonstrated in bone, collagen, elastin and the synthetic bone mineral hydroxyapatite. Piezoelectric coefficients exhibited by these biological materials are generally low, limiting technological applications. Research guided by quantum mechanical calculations has changed this situation, with the demonstration that the amino acid crystal β-glycine possesses a piezoelectric coefficient similar in magnitude to materials such as barium titanate or lead zirconate titanate that are in commercial use.

(b) Molecular and nanomaterials

The expansion of computational power, the development of better/faster characterization methods and the evolution of self-assembly and supramolecular chemistry have enabled the dream of 'materials by design' to approach fruition. This 'materials design revolution' is poised to profoundly influence society by impacting, amongst other matters, energy sustainability and drug development. Simply put, by finding the right chemistry, materials scientists and engineers can gain the level of power that architects have when they design new buildings. Crystalline materials by design – crystal engineering – is one of themes of this cluster.

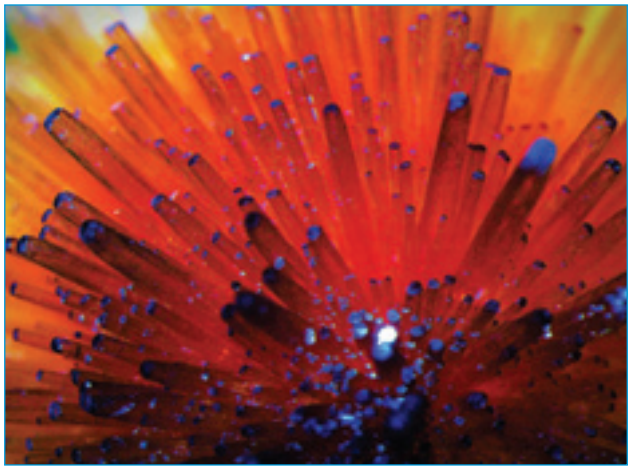

Figure 4: 'Skyscrapers' – an image of crystals of coordination polymers taken by Bernal Institute post-graduate student ***Shi-Qiang Wang****. This image was awarded a prize in the Crystal in Art Virtual Competition 2020 of the BACG. Photograph courtesy M.J. Zaworotko.*

Bernal Chair of Crystal Engineering Prof. Michael Zaworotko leads the crystal engineering research group that he established upon joining UL in 2013. Crystal engineering is enabled by one of Bernal's legacies: the Cambridge Structural Database, CSD. The CSD was proposed by Bernal[13,14] and constitutes perhaps the first scientific database. There are two main areas of study in the crystal engineering group: advanced porous materials and multi-component pharmaceutical materials. Recent highlights include articles in *Science* in 2016 and 2019 that dealt with improving the energy efficiency of ethylene purification, the largest volume product of the petrochemical industry. Dr Matteo Lusi leads a research group that studies mixed crystals – solid solutions of two or more molecular compounds that are characterized by structural disorder that enables variation of stoichiometry in continuum. Often such variation results in modulation of structural and physicochemical properties which in turn facilitates fine-tuning of bulk properties. Such behaviour is particularly important in pharmaceutical, agrichemical and optoelectronic materials. Prof. Kevin Ryan leads a team that studies colloidal nanocrystals with particular emphasis on semiconductor nanorods and their device scale assembly by directed (electric fields) or non-directed approaches for scalable applications in photovoltaics. The team has pioneered routes whereby the nanorods can be assembled from solution such that each rod is vertically aligned and close-packed. A second work programme addresses low cost solution synthesis of silicon and germanium nanowires by seeded and non-seeded strategies, targeted particularly towards generating wires in high yield. Control over nanowire length for the formation of nanorods was achieved by a modification of this synthesis protocol.

(c) Timepix and 3D Electron Diffraction

Dr Andy Stewart leads a 3D Electron Diffraction group. Structure determination of nanocrystals of organic pharmaceutical compounds by 3D Electron Diffraction (3DED) at room temperature is possible using the Timepix direct electron detector with increased quantum detection efficiency[15]. A convolution of the electron density and the nuclear charge makes it possible to determine the position of hydrogen atoms in structures without the need to grow millimetre sized crystals for neutron diffraction studies. It is hoped that the ability to investigate nano-sized crystals will answer the question of why

so few crystal polymorphs are currently observed despite the many possible based on crystal structure predictions. Is it a question of kinetics – the crystals cannot be grown to sufficiently large size or in sufficient numbers to be used in X-ray studies? It is hoped that the fast developing field of 3DED will help reveal the deeper crystal physics behind this question.

Until recently, structure determination of organic compounds by transmission electron microscopy required data collection at liquid-nitrogen temperatures to reduce the effects of radiation damage. The novel Timepix detector combines a high dynamic range with a very high signal-to-noise ratio and single-electron sensitivity, removing the need to freeze the specimens to obtain data good enough to enable *ab initio* phasing of beam-sensitive organic compounds. Low-dose electron diffraction data ($\sim$0.013 e^{-} $Å^{-2}$ s^{-1}) collected at room temperature were of sufficient quality for structure determination using software developed for X-ray crystallography which includes the appropriate electron scattering factors.

The Stewart group has show that 3DED coupled with a sensitive Timepix detector allows fast and efficient three-dimensional crystal structure analysis of organic pharmaceutical compounds at room temperature. The technique will allow higher-throughput examination of nanometre-sized samples in a transmission electron microscope complementing standard single-crystal and powder X-ray diffraction. The recent advances in 3DED have led to an interesting new question for crystallography. Electron microscopes are sensitive enough to observe the transition from nucleation to particles and onto crystals during the growth process. This raises the question as to how many unit cells are sufficient to produce an observable crystal, the structure of which can be determined by 3DED methods. This question is particularly pertinent for crystal growth and phase change materials. Currently the International Union of Crystallography's definition of a crystal does not provide a quantitative number to declare an object as a crystal. The Stewart group has been working on this question (a talk on this was given at the 2021 BCA-BACG Spring Meeting[16]) and will be shortly publishing a paper suggesting a methodology to quantitatively define an object as crystalline.

(d) Process Engineering

Prof. Gavin Walker leads the Process Engineering Cluster, which is aligned to UN Sustainable Development Goals in Health, Energy and the Environment/Sustainability. Improving population health and well-being is critically dependent on the development of new biopharma solutions, which in order to complete the drug approval process and have maximum impact must be amenable to scalable processing and manufacture, this often demanding innovative processing. Ensuring access to affordable, reliable, sustainable and modern energy for all will require a substantial increase in the share of renewable energy in the global energy mix. Advanced energy storage solutions are sought and can help here through C-storage/conversion but so too can process synthesis and integration. Fostering and supporting responsible consumption and production ensuring sustainable consumption and production patterns can reduce waste generation through prevention, reduction, recycling and reuse. Reduced solvent waste can be achieved through solvent-free processing of advanced materials and through multiphase, bio-, and hybrid processing.

(e) Composite Materials

Prof. Paul Weaver leads this cluster, a major aim of which is to help develop new industry in Ireland based on new intellectual property. To meet this aim the cluster focuses on two main application areas: renewable energy and sustainable aircraft transport. Research involves a combination of materials development, manufacturing technology and design methods where each will be pursued in balance and harmony with one other so that equi-fidelity contributions to technology are made. In terms of renewable energy, Dr Maurice Collins leads a research programme pursuing the development of new carbon fibre materials from sustainable resources (lignin). Once large scale production of these materials is achieved, composite materials will be developed using thermoplastic matrices from natural, sustainable supplies. Research in manufacturing and design methods both contribute in a complementary manner to application areas such as renewable energy and sustainable transport. A research focus of the cluster is on the development of methods of manufacturing composites that will help reduce the cost of energy for wind turbine blades and lead to cheaper, better-performing aircraft (less fuel burn). Design methods will focus on advanced stress analysis development and subsequent tool development that exploits our new combination of materials and manufacturing technology.

Concluding remarks

The future focus of the Bernal Institute is likely to include, in addition to current themes, areas such as sustainability in food, energy and water, three areas of application where the Institute has growing momentum. It seems inevitable that the structure-function relationships of crystalline and non-crystalline materials that inspired Bernal will continue to guide its direction. We are now at the stage where crystal engineering can have major positive impact on our future. Engineered crystals that can efficiently separate mixed gases and abstract specific molecules from the atmosphere have been demonstrated. An application of this technology with obvious world-saving potential is one step separation of CO_2 from the air at ambient temperature and pressure to combat global warming. Another crystal engineering system currently under trial could help solve the developing world's need for potable water by direct extraction from the atmosphere (these last two projects were described in Michael Zaworotko's Plenary talk at the 2021 BCA-BACG Spring Meeting[16]).

The field of crystallography has expanded enormously since the 1920s when Bernal commenced his pioneering research at Cambridge elucidating the structure of life's molecules using XRD. A century later, it is clear that crystals and the science of crystallography will continue to expand the social function of science to create a more equitable and harmonious society. With what has already been achieved and the exciting future prospects, we may, with good reason, hope that crystals are going to play a major role in saving the world.

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Acknowledgements

I would like to acknowledge contributions to this article by Prof. Kieran Hodnett, Prof. Edmond Magner, Prof. Michael Zaworotko, Dr Matteo Lusi, Dr Tofail Syed. Prof. Tewfik Soulimane and Dr Andrew Stewart, all of whom gave freely of their time and support. Jon O'Halloran, BI Operations Manager, has also been most supportive.

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SARS-CoV-2-related structures in the Protein Data Bank

WITH the March 3 update of the PDB, over one thousand SARS-CoV-2-related structures are now freely available in the PDB.

The first SARS-CoV-2 structure, a high-resolution crystal structure of the coronavirus main protease (PDB **6lu7**), was released early in the pandemic on February 5, 2020. Since then, structural biologists have determined the structures of most of the proteins in the SARS-CoV-2 proteome, including the spike protein binding to its ACE2 receptor and neutralizing antibodies, and the main protease, the papain-like proteinase, and other promising drug discovery targets. All of the structures and related data are available for exploration from dedicated pages on wwPDB partner websites: RCSB PDB, PDBe, PDBj, and BMRB.

Rapid public release of SARS-CoV-2 structures has greatly increased our understanding of Covid-19, allowed direct visualization of emerging variants of the virus, and facilitated structure-guided drug discovery and reuse to combat infection. Open access to PDB structures has already enabled design of effective vaccines against SARS-CoV-2.

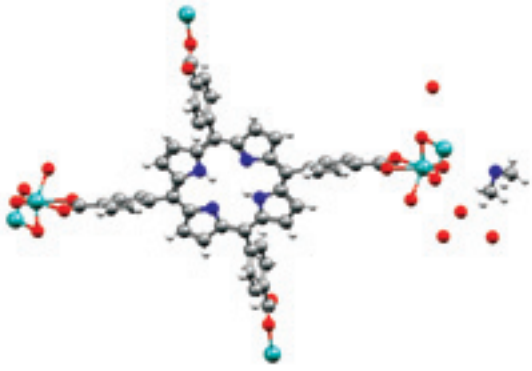
The response of the research community to the pandemic has highlighted the importance of open access to scientific data in real time. The wwPDB strives to ensure that 3D biological structure data remain freely accessible for all, while maintaining as comprehensive and accurate an archive as possible.

The impact of these over one thousand structures, and many more coronavirus protein structures to come, stands as a testament to the importance of open access to structural biology research data.

John Berrisford
European Bioinformatics Institute

MOF data set provides 10k structures free for academic research

THE Cambridge Crystallographic Data Centre (CCDC) has made around 10,000 metal-organic framework structures free to academics in the new CSD MOF Collection.



The Collection includes the crystal structure data for 10,636 MOFs from the Cambridge Structural Database (CSD). The data are provided as single-block CIF files along with CSV indexes, allowing researchers to search and view the structures, or apply analytical or learning techniques to the data. The collection has been built to provide a simplified and focused data set for computational research including just the 3D porous frameworks, rather than the complete collection of 107,980 MOFs in the full CSD with all the user-led filtering options available in the CSD Software Portfolio.

To build the collection, the CCDC worked with researchers at the University of Cambridge Department of Chemical Engineering and Biotechnology. Here the molecular mechanisms and applications surrounding porous materials like MOFs are researched, including their use in drug delivery systems, hydrogen storage and carbon capture.

The CSD MOF Collection is available to download now from www.ccdc.cam.ac.uk.

BCA Spring Meeting 2022

PLANNING is at an advanced stage for the 2022 BCA Spring Meeting to be held in Leeds, so please put the dates in your diaries. Details and titles for sessions are given below to inspire you to start thinking about contributing oral or poster abstracts. Remember that the abstract deadline early in the New Year always seems to arrive sooner than expected…

Session Details

Monday 11th April, 2022

Young Crystallographers Group (YCG)

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography, from across the BSG, CCG, PCG and IG, to present their work in a supportive and friendly environment, which will be run by fellow early career scientists.

YCG Opening Plenary

Dr Claire Hobday *(University of Edinburgh)*

Session Chair: Dr Tom Roseveare, University of Sheffield

YCG Research Sessions

Contributed talks from the YCG community.

(Session 1 Chair: Dr Tom Roseveare, University of Sheffield)

(Session 2 Chair: Dr Natalie Pridmore, University of Bristol)

(Session 3 Chair: Aly Abdeldaim, ISIS Neutron and Muon Source/University of Birmingham)

(Session 4 Chair: Dr Charlie McMonagle, European Synchrotron Radiation Facility)

Flash Poster Presentations

Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide.

Session Chairs: Dashnor Beqiri, University of Warwick and Lee Birchall, University of Kent

Tuesday 12th April, 2022

Parkin Lecture – recipient tbc

Session Chair: Dr Rachel Wilkinson, Swansea University

YCG Closing Plenary

Dr Sam Horrell *(Diamond Light Source)*

Session Chair: Dr Charlie McMonagle, European Synchrotron Radiation Facility

Lonsdale Lecture

Prof. Andrew Goodwin *(University of Oxford)*

Disorder by design: from form to function

Session Chair: Dr Tom Roseveare, University of Sheffield

PCG Plenary

Prof. Xiaodong Zou *(Stockholm University)*

Electron crystallography: past, present and future

Session Chair: Dr Alex Gibbs, University of St Andrews

Sessions 14:20 – 15:50

PCG: Porous Materials

Session Chair: Aly Abdeldaim, ISIS Neutron and Muon Source/University of Birmingham

BSG: RNA-Protein Interactions

Session Chair: Prof. Phil Evans, University of Cambridge

CCG: Crystallography under extreme conditions

Session Chair: Dr Charlie McMonagle, European Synchrotron Radiation Facility

Sessions 16:35 – 18:05

PCG: Structure property relationships in energy storage

Session Chair: Dr Karen Johnston, University of Durham

BSG: Correlated tomography

Session Chair: Dr Maria Harkiolaki, Diamond Light Source

CCG: Nucleation & Phase Changes

Session Chair: Dr Katharina Edkins, University of Manchester

CCG Plenary

Prof. Michaele Hardie *(University of Leeds)*
Supramolecular cages and networks with pyramidal ligands
Session Chair: Dr Michael Probert, University of Newcastle

Wednesday 13th April, 2022

IG Plenary

TBC
Session Chair: TBC

Sessions 10:15 – 11:45

PCG/CCG: Advances in complementary techniques and *in situ* crystallography

Session Chair: Dr Hamish Yeung, University of Birmingham

BSG: Electron Diffraction

Session Chair: Dr Peijun Zhang, Diamond Light Source

IG: Metallurgical Crystallography

Session Chairs: Judith Shackleton and Dr Helen Blade, AstraZeneca

Sessions 15:30 – 17:00

YCG+ Careers Session

An opportunity to hear from and pose questions to the panellists about their jobs and career paths, in various fields of crystallography.
Panellists: tbc
Session Chairs: Dr Natalie Pridmore, University of Bristol and Tom Roseveare, University of Sheffield

BSG: Membrane Proteins

Session Chair: Dr Julien Bergeron, King's College London

IG: *In situ* crystallography – looking inside the black box

Session Chairs: Judith Shackleton and Dr Helen Blade, AstraZeneca

Hodgkin Lecture:

Elspeth Garman *(University of Oxford)*
Macromolecular Crystallography in 112 AD (After Dorothy)
Session Chair: Prof. Richard Cooper, University of Oxford

Thursday 14th April, 2022

BSG Plenary:

TBC
Session Chair: TBC

Sessions 10:15 – 11:45

PCG: Poorly crystalline solids (PDF)

Session Chair: Dr Arianna Minelli, University of Oxford

BSG: RT data collection

Session Chair: Dr Allen Orville, Diamond Light Source

CCG: Tricks of the trade – from crystallisation to publication

Session Chair: Dr Claire Wilson, University of Glasgow

Sessions 12:00 – 13:30

PCG: Functional materials

Session Chair: Dr Paul Saines, University of Kent

BSG: Covid Drug Discovery

Session Chair: Dr Daren Fearon, Diamond Light Source

CCG/BSG: Understanding Crystallization through Diffraction and Complementary Methods

Session Chair: Prof Joop ter Horst, University of Rouen

CLOSE OF CONFERENCE

Chemical Crystallography Group Autumn Meeting

THE BCA Chemical Crystallography Group (CCG) are hosting their Autumn Meeting on Wednesday 24th November 2021. The event will run over one day and will be held in a virtual format.

The theme of the meeting will be 'Crystals out of Equilibrium', with a range of speakers looking at dynamic crystals and processes, functional properties and metastability of crystalline materials. The meeting will start at 10.00 a.m. (UK time) and finish at 4.30 p.m. We are hoping to host an online social event afterwards.

Please go to the CCG website https://ccg.crystallography.org.uk/ to find the latest information on this as well as the speaker line-up and details of how to register.

We will be charging a small registration fee of £10 to cover the costs of technical assistance and to support the scientific endeavours of the CCG.

We look forward to seeing you all (virtually) in November

Helena Shepherd for the CCG Committee
University of Kent

18th BCA/CCG Intensive Teaching School in X-ray Structure Analysis

12th-17th April 2021 – Online

THE last year has seen us all becoming very familiar with virtual meetings and the 18th BCA/CCG Intensive Teaching School in X-ray Structure Analysis, 12-17th April 2021, was no exception. Approximately one third of the 84 students came from outside the UK with representation from 12 different countries: UK, Brazil, China, Croatia, Finland, France, Germany, India, Ireland, Mexico, Switzerland and the USA. Clearly the difference in time-zones meant some people had to be up either very early in the day or very late into the night to join in with the school. We are very grateful to those students for adjusting their day to participate fully in the school!

The content and format of the biennial course is designed to provide students with the opportunity to gain a good theoretical understanding of various aspects of crystallography from a single crystal perspective. The course consists of a mixture of lectures and small group tutorials designed to help students improve their understanding of the lecture material. The online nature of the course this year meant some changes were made to the course format designed to try and avoid online fatigue. We had a virtual learning environment containing supporting material for the lectures and course as well as discussion forums. Prior to the start of the course the students watched some pre-recorded maths lectures and completed some pre-work designed to give them a good grounding in the maths used throughout the course. This meant that the course could run over 6 days with lectures from **Professor Simon Parson**, **Dr Lukas Palatinus**, **Dr Andrew Bond**, **Dr Helena Shepherd**, **Dr Richard Cooper** and **Dr Mark Senn**, who guided the students through the following topics over the course of the week; Symmetry, Data collection, Fourier/Patterson, Charge Flipping, Electron Diffraction, Superspace, Direct Methods, Parametrisation, Least Squares, Refinement, Derivation of Results and Twinning.

This year we increased the number of tutors to allow for smaller tutorial groups, giving 14 tutor groups of 6 students. We welcomed three new tutors, **Dr Samantha Chong**, **Dr Matic Lozinsek** and **Dr Jeremiah Tidey** who bravely took on tutoring for the first time online, and we were pleased to have **Dr Roy Copley** and **Dr Mark Warren** return after a break from tutoring. We also welcomed back tutors from the 2019 school **Dr Christine Beavers**, **Dr Andrew Cairns**, **Dr Laszlo Fabian**, **Dr Nick Funnell**, **Dr Claire Hobday**, **Dr Iain Oswald**, **Dr Amber Thompson**, **Dr Claire Wilson** and **Dr Hamish Yeung**. We all became more familiar with the use of breakout rooms and document viewers! However, this seemed to work well for switching between lectures and tutorials and we were delighted to see that the feedback from the students was overwhelmingly positive.

The evening sessions included a quiz run by **Professor Richard Cooper**, which resulted in a tight result with three teams being within one point of one other. A crystallographic panel hosted by **Dr Helena Shepherd** was very well received, giving the opportunity for the students to pose questions on any crystallography-related topics from job opportunities to applying for beamtime, or how to carry out certain types of refinement. We also had a session on Databases run by **Dr Pete Wood**, **Dr Ilaria Gimondi** and **Dr Suzanna Ward** at the CCDC and talks on Synchrotrons (**Dr Christine Beavers**) and Neutrons (**Dr Mark Senn**) all of which generated significant interest from the students.

This year we were also keen that people didn't spend the whole week inside in front of their computer so held a distance challenge between the school staff and students. Everyone participating input the distance of any walks, runs and cycling trips that they fitted in during the week, with runs and bike ride distances scaled to make them comparable to walking. Overall, 17 staff (lecturers and tutors) and 30 students covered over 500 miles during the week, with the student team just beating the staff with 277.5 miles versus 242 miles.

The final afternoon saw announcement of the winners of the bar quiz and distance challenge. It was also a chance to thank the people who had contributed to the success of this year's school: the course director (**Professor Richard Cooper**), course notes preparation (**Dr Claire Wilson**), organisers (**Professor Judith Howard** and **Dr Hazel Sparkes**), lecturers, tutors and students. We were also very sad to say goodbye to **Professor Simon Parsons** who has stepped down as a lecturer, having been an integral part of the school for over 20 years working as a tutor, lecturer and course director. He will be very sorely missed as he has supplied considerable enthusiasm, knowledge and lots of fun throughout his time in the school.

Following on from the school there was an optional online Olex2 workshop run by **Dr Horst Puschmann**, **Dr Oleg Dolomanov**, **Dr Florian Kleemiss** and **Dr Florian Meurer**. This was attended by 55 registered participants and was very well received. Participants had the chance to learn how to use Olex2, with a combination of talks, demos and question and answer sessions.

Hazel Sparkes (Local Organiser)
Bristol University

Protein structures to get one's teeth into

AS well as being a place for early career researchers to discuss their recent research, the YCG satellite meeting has often involved lively discussion about public engagement. This is, in part, due to the programme including the Parkin Lecture. This annual prize lecture, named in honour of Dr Andrew Parkin, is an opportunity for a member of the YCG community to discuss their recent experience in delivering and developing public engagement activities.

Typically, the Parkin Lecture has offered new perspectives on educating a wider community and inspired further discussion at the meeting. In the 2021 Spring Meeting, this was no different with the lecture being presented by **Elizabeth Driscoll**. Elizabeth shared her experience of developing resources both before and during the pandemic. Her development of engagement activities based on battery research was outlined in a recent Chemical Education article.[1] Elizabeth was also awarded the RSC 2021 Inspirational Member Award for this work. During her Parkin Lecture Elizabeth stressed the importance for ensuring that the resources you produce are suitable for all. This led her redeveloping her models using colour and tactile features to make them more suitable for people with visual impairments. A new approach in developing tactile resources has been, recently, reported by **Bryan Shaw** and co-workers at Baylor University.[2]

The team at Baylor University noted that mouthfeel was an underutilised tactile learning tool, particularly in the context of visual impairment. This prompted the group to develop a series of 3D protein molecules made from either non-toxic resin or edible gelatine, the shape of which could be explored using a participant's mouth. These candy-sized protein structures were as easily identified by mouth as identifying a structure from a 3D animation, but the added possibility of coding structures with flavour brings added potential to these edible resources.

This recent paper has started me thinking how future engagement activities could be developed with all the senses in mind. Too often I consider the visuals to be the most important aspect of educating an audience, but perhaps feel, taste and smell would be as/more valuable in informing an audience of a scientific concept.

The YCG are always keen to hear about new approaches to public engagement. If you have an early career researcher that has been actively involved in developing and delivering teaching/public engagement activities, please consider nominating them for the Parkin Prize Lecture. For more information visit https://ycg.crystallography.org.uk/prizes/.

Tom Roseveare
University of Sheffield

References:

1. E. H. Driscoll, E. C. Hayward, R. Patchett, P. A. Anderson and P. R. Slater, *J. Chem. Educ.* **97**, 2231–2237 (2020). (https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00282).
2. K. M. Baumer, J. J. Lopez, S. V. Naidu, S. Rajendran, M. A. Iglesias, K. M. Carleton, C. J. Eisenmann, L. R. Carter and B. F. Shaw, *Sci. Adv.* **7**, 1–13 (2021). (https://advances.sciencemag.org/content/7/22/eabh0691).

South West Structural Biology Consortium Meeting 2021

14-15 July 2021 – Virtual

THE meeting opened with a plenary talk given by Peijun Zhang (Oxford) on *HIV-1 capsid curvature and its interaction with host cell factor* and chaired by Ivo Tews (Southampton). Peijun was studying the conical shaped HIV-1 capsid. Her group made an all-atom model of the HIV-1 capsid (216 hexamers +12 pentamers) – the largest ever simulation on supercomputer which showed the general structure of the capsid. Electron diffraction studies on fibres made up of the hexamers diffracted to 8Å and showed that different widths of fibres relate to different curvatures of capsid. They finally got to 3.6Å in a cryoEM study of the fibres by adding CypA. Those data showed that the hexamer is intrinsically curved – not planar as suggested by the crystal structure – which showed how the curved capsid is formed, i.e. by the bent hexamers and not by planar hexamers at angles to one other. They then used cryoET to study whole capsids, but had problems with high background from protein floating around in the cell. This was solved by adding a pore-forming molecule to reduce background, allowing the excess multimers to be released. Lastly, using subtomogram averaging with addition of CypA and IP6, they could see hexamers and pentamers at around 6-8Å. Both hexamers and pentamers bind IP6 at their centre, but it was found that the pentamer binds IP6 stronger than the hexamer. The CypA, which is highly conserved, promotes infection of HIV-1 and other viruses. It was found to bind the HIV1 capsid *via* a CypA-binding loop, promoting curvature by binding at two points either bridging 2 hexamers or 3 hexamers.

The first session of talks was chaired by **Lavinia Gambelli** (Exeter) and started with **Alicia Teijeira Crespo** (Cardiff) talking about the *Structure of ChAdOx1 Vaccine.* ChAdOx1 is a Chimpanzee Adenovirus developed by Oxford University. It had been engineered to express the SARS-Cov-2-5 surface glycoprotein and was found to induce robust immunity, but also induces VITT (thombolytic disease). CryoEM gave the structure of the overall capsid to 4.2Å, but didn't show the all-important fibre knob. Therefore, they moved to crystallography, and managed to get the structure to 2.0Å. They then investigated two binding partners CAR and PF4. CAR is a high affinity receptor for ChAdOX1, but doesn't bind CD46. The PF4 binding was found to be probably due to electrostatic interactions and they tested this with dynamics simulations. The next talk was from **Alex Neuhaus** (Exeter) and entitled *CryoEM reveals two distinct type IV pili assembled by the same bacterium*. Type IV pili are long filaments, assembled by a multi-component machinery. They can be retracted rapidly with high forces (>100pN) and are essential for pathogenicity. Initial CryoEM images showed two different types of filaments which could be sorted easily into two groups. They solved both to around 3.3Å. The structures indicated that two different proteins are making these pili, when there should be only one available. One was shown to be PilA4 as expected, while the other was PilA5. Extra density in the maps could be ascribed to glycosylation. Using knockout systems they showed that the different pili have (partly) different functions. Using known structures and other biochemical information they were able to make a reasonably complete model of whole machinery. The final talk was given by **Patricia Gil Diez** (Exeter) on *Structure of the eukaryotic hibernating ribosome dimer from the microsporidia Spraguea lophii*. Microsporidia infect a wide variety of hosts and are a threat to the global food chain (honey bee colonies, fish farms). The spores have a polar tube to inject host cells with infectious material. However, some complexes injected are larger than the diameter of tube, so it is not obvious how this injection happens. Using subtomographic images they could see ribosomes in the polar tube that appear to form dimers. This is known to happen in other spores, and the ribosomes use a co-factor to stabilise the dimer and keep it inactive. Images show that the microsporidia dimer is structurally different from normal dimerization, and also there is no known co-factor, though it is thought that the dimerization is also to keep the ribosomes inactive. CryoEM at 2.5Å of the ribosomes (monomer only – the dimer is not stable) gave the structure. Extra density in the models was attributed to tRNA and the L1 stalk.

The second session chaired by **Bruce Lichtenstein** (Portsmouth) started with **Charlotte Cordery** (Southampton) giving a talk entitled *Phylogenetic analysis with prediction of cofactor binding for Psudomonas aeruginosa (PA) PAS domains*. PAS domains are intracellular sensory domains that often bind cofactors. CACHE domains are a subset of PAS domains that can be periplasmic or extracellular. PA can switch between planktonic and biofilm forms, depending on PAS domains to sense the levels of cyclic di-GMP. The group used phylogenetic analysis (HMM) to discover more PAS domains in PA (finding 102) and to study their architecture. They grouped these on sequences by maximum likelihood phylogeny and analysed expected pockets with CASP1. They also analysed conserved residues to highlight which were likely to be ligand binders and to predict their behaviours. The next talk from **Alessandro Agnarelli** (Sussex) was on *Analysing IRF-4 interactions to ISRE motifs in Multiple Myeloma*. Multiple Myeloma (MM) is an aggressive and incurable cancer. IRF4 is central to the genesis of MM and knockdown of IRF4 shows a dramatic decrease in MM. There are no current inhibitors for this molecule. IRF4 can heterodimerise with ETS or AP-1 to bind to different DNA sequences, or it can homodimerise and bind a GAAA sequence (called ISRE sequence). IRF4 has low affinity to DNA, so does it dimerise or bind to other proteins to enhance this? The group studied binding to various ISRE sequences and found that the upstream sequence is important for affinity. Crystallography with the canonical sequences though show no protein dimerisation (molecules are on opposite sides). Finally, **Jenn-Yeu Alvin Szeto** (Bristol) spoke on *Characterising the structural and biophysical interactions between nonsense-mediated mRNA decay factors UPF2, UPF3B and RNA*. There are three quality control pathways for mRNA translation, one of which is NMD. This utilises Up-Frameshift Proteins (UPFs) to interact with the RNA. To facilitate crystallographic studies UPF2 was tested against various RNA molecules. UPF2 was found to have the highest affinity to ssRNA, to need at least 13 nucleic acids and has a pyrimidine preference. Crystals were obtained from the Nucleix (Qiagen) suite. They also showed that UPF3B preferentially binds RNA when UPF2 is present in a 1:1:1 complex, and they studied this complex with cryoEM.

The last session of the day was chaired by **Michael Zahn**

(Portsmouth) and the first speaker was **Alex MacPherson** (Bath) on *The allosteric modulation of C5 by knob domain peptides*. Ultra-long complementarity-determining regions (CDRs) have a knob domain that could be used as an ultra small antibody. The group were looking for immune-derived peptides against C5 from bovine sources and could show that isolated knob domains bind C5 with high affinity. Functional assays revealed three distinct mechanisms – the K8 and K92 classical allosteric pathway and the K57 alternative pathway. Crystal structures were solved for all types. These knob domains could be made by chemical synthesis, which allowed a much larger library to be easily constructed, even including non-native amino acids to improve stability. **Lynden Rooms** (Bristol) then spoke on *Structural and functional insights into PabB – the cellular target of abyssomicin C*. Abyssomycins are novel antibiotics derived from the actinomycete *M. maris*. Abyssomicin C binds to and inhibits PabB (which is on the chorismate pathway) – the first natural product to do so – by binding irreversibly to a cysteine residue in the active site. It was also found to inhibit TrpE (tryptophan biosynthesis pathway (96% identical to PabB)). The group have managed to get X-ray structures of both enzymes in native conformation and are now trying to get the ligand- bound versions. The last talk of the day was given by **Daniel Hinchen** (Portsmouth) on *Engineering a cytochrome P450 for demethylation of lignin-derived aromatic aldehydes*. Lignin is the most common aromatic biopolymer on the planet, and also is a waste product of the food and biofuel industries. Heterogeneity is the primary challenge for efficient valorisation of lignin. Initial degradation produces many aromatic compounds with different side groups which then need to have their aromatic rings cleaved, a key step for further downstream processing. Before this, all rings need to be deoxymethylased, which can be done by GcoAB, a two-component Cytochrome P450. The problem with this enzyme is that it will bind a wide range of substrates, but doesn't turn most over, becoming stuck in the process. The group used structure-based engineering to improve activity with non-native substrates and managed to get crystal structures to high resolution with some of these.

The second day opened with a plenary from **Daren Fearon** (Diamond Light Source DLS) on *Crystallographic Fragment Screening with the XChem platform at DLS and hit-to-lead progression of novel SARS-CoV-2 Main protease inhibitors*, and was chaired by **Ivo Tews** (Southampton). The fragments are small molecules (< 500Da) that can be bound with low affinity to a target protein. If two fragments bind at close proximity then they can be grown into larger, higher affinity, novel inhibitors. NMR, SPR or X-rays can be used for fragment screening. The benefit of X-rays is the very high sensitivity (>=10mM) of binding. The technique also gives immediate structural information, but does require a robust crystallisation protocol to provide up to 1000 identical crystals for fragment soaking. Due to success of XChem, five other similar systems are being setup at other synchrotrons. Fragments are added to each drop by acoustic dispensing with an ECHO. Each crystal is mounted and cryocooled using the crystal shifter system and data is collected completely automatically at a rate of ~30/hour. Data is analysed using Pandda in the XCE workflow gui. The Pandda software allows very weak hits to be found against an average background of unbound datasets. The hits can then be passed to the Fragalysis software for further elucidation. For Sars-CoV-2, vaccination is underway, but antivirals will still be useful for those that cannot be vaccinated. Repurposing of known drugs has so far proved unsuccessful. The group ran eight Covid-19 proteins through XChem, with all data posted on Zenodo and bioRxiv. The main protease (Mpro) is a cysteine protease responsible for polyprotein processing. Its structure was solved in January by a Chinese team. XChem was completed on this target in under 3 months with 78 fragments found, a large proportion of which bound in the active site. This was the start of the Covid Moonshot – a worldwide collaboration of over 30 groups. Initial hits were made by growing/combining fragments and getting micromolar hits. Further elaboration made inhibitors down to <100nM binders, which also showed activity against viral particles. Lead optimisation is continuing to improve the metabolic stability and oral availability of the inhibitor.

The first session of the morning was chaired by **Ben Bax** (Cardiff) and started with a talk by **Xiangrong (Tina) Chen** (Sussex) on *Uncovering an allosteric mode of action for a selective inhibitor of human Bloom syndrome protein*. Bloom Helicase is a member of the RecQ helices family and is important in cancer. The search for inhibitors started from known helicase inhibitors and tested these against Bloom. Five compounds were found to have activity. After excluding false positives, three series were selected for further elaboration. Compounds were tested against ATPase and MST assays. Series C was found to bind when ss-DNA was present, but not when nucleotide only was present; thus this was binding in an allosteric site. After many protein constructs were tested, they eventually managed to get an X-ray structure with the compound and DNA, showing the pocket that the inhibitor was occupying. With the inhibitor bound, the aromatic rich loop (conserved among RecQ helicases) is remodelled and blocks the conformational changes required for catalytic activity. This is a highly selective inhibitor of Bloom. The second talk was given by **Kirsty Goudar** (Bristol) on *Substrate and inhibitor interactions of Class D OXA b-lactamase*. β-lactams are currently the most highly prescribed antibiotics. β-lactamases break down these antibiotics, so inhibitors for these would be very useful. There are four classes, three serine and one metallo, with over 250 types of OXA lactamases. The work described concentrated on the OXA48 type (of which there are still over 80 types). These are the most prevalent in the community and can break down all current antibiotics. The group were concentrating on two, OXA163 and OXA405. These only have small changes in loops, but interact differently to substrate. The group have managed to get the first X-ray structures to high resolution of OXA48-like enzymes with ertapenem, meropenem and avibactam. The final talk in the session was given by **Sumita Roy** (Exeter) on *A structural and mechanism insight into the mechanism of ROK kinases.* Sugar kinases are used to produce various sugars from carbohydrates. NagK is a ROK (repressor, open reading frame, kinase) and phosphorylates monosaccharides (specifically GlcNAc). This protein is an attractive target for inhibition to target bacteria that rely on the cell wall for the pathogenesis process. They used a coupled ATP assay to study the enzymatic action, and showed it to follow a sequential mode, GlcNAc binding first, then ATP. Metal binding was shown to be important for activity and proved to work best with Mn^{2+}. X-ray structures to 1.8Å were obtained for apo, GlcNAc bound, and GlcNAc and AMP-PNP bound. When GlcNAc binds there is a 23° rotation of domains compared to the apo.

The last session of the meeting was chaired by **Jean van den Elsen** (Bath). The first talk was from **Becky Connors** (Exeter) on *CryoEM structure of the outer membrane secretin channel pIV from the f1 filamentous bacteriophage*. The Ff family of filamentous phages are very simple organisms – only 11 genes, useful for biotechnology, vaccines and phage display techniques. Phage forms a tight pore to let phage particles out, so the cell doesn't lyse, allowing the cells to carry on living and produce more phage. f1pIV is one of the proteins involved

in the pore. A CryoEM map to 2.7Å showed a 15-fold multimer, forming a 60 strand double-walled beta-barrel. There are two mobile loops that close the pore when not in use. When open, the pore has a diameter of 65Å, large enough to accommodate the phage particle. It has structural similarity to bacterial secretins. The next talk was from **Neeleema Seetaloo** (Exeter) with *Synuclein plasticity: the Achilles heel to the onset of Parkinson's disease*. Parkinson's is characterised by Lewy bodies in the neurons. In the disorder, the non-structured protein α-synuclein (aSN) aggregates from a monomeric state to multimeric fibrils. aSN is found in extracellular, intracellular and lysosomal spaces. NMR, specifically amide hydrogen-deuterium exchange (HDX), was used to analyse the aSN structure in these spaces. It was found that the aggregation had distinct kinetics in each space, the C-terminus strongly influencing the aggregation and the N-terminus and hydrophobic core strongly influencing the elongation of the fibril. The last talk was given by **Charlotte Collingham** (Reading) on *Novel bile acid derivatives as potential drugs for neurodegenerative disease*. Mitochodria are the powerhouse of the cell and dysfunctional mitochondria are at the heart of many diseases. Several pathways involving mitochondria are involved in Parkinson's. UDCA (a bile acid) has been identified as a therapeutic option for neurodegenerative diseases. The hypothesis is that restoring key lipid levels will help reduce neurodegeneration. Novel bile acid derivatives were tested to see their effect on mitochondrial function (trying to restore ATP levels, ROS levels, lipid levels). BioGPS was used to identify targets for the novel bile acid derivatives. One of these targets transports mitochondrial lipids. It is a heterodimeric protein and the bile acid derivatives are thought to interact with a loop (Ω-lid) to enhance interactions with the lipids. The yeast homolog of this protein was expressed, purified, crystallised and the structure solved to 1.9Å with a best-in-class bile acid derivative bound.

The winners of the talk prizes were: **Neeleema Seetaloo**, **Alex Neuhaus** and **Alex MacPherson**.

There were also four software talks: **Kyle Stevenson** (CCP4) on *CCP4i2*, **Eugene Krissinel** (CCP4) on *CCP4Cloud*, **Colin Palmer** (STFC) on *CCPEM* and **Vicky Higman** (Leicester) on *CCPNmr Analysis Version-3: modern software for integrated NMR analysis*.

The posters presented were:

1) **Rachael Andrews** (Bath) on *Synthetic cannabinoid receptor agonists (SCRAs) as Monoamine Oxidase-A specific inhibitors*.
2) **Rachel Bolton** (Southampton) on *Measuring energy-dependent photoelectron escape in micro crystals*.
3) **Becky Connors** (Exeter) on *CryoEM structure of the outer membrane secretin channel pIV from the f1 filamentous bacteriophage*.
4) **Charlotte Cordery** (Southampton) on *Phylogenetic analysis with prediction of cofactor binding for Pseudomonas aeruginosa PAS domains*.
5) **Raul Cioaca** (Reading) on *In silico biomolecular docking studies of the Farnesoid X Receptor (FXR) DNA binding domain reveal structural reasons underpinning isoform-specific DNA binding*.
6) **Kain van der Elsen** (Exeter) on *The structural basis of +ssRNA virus replication*.
7) **Anatol Gawrzak** (Reading) on *Identification and development of prebiotic targets in the gut microbiome*.
8) **Kirsty Goudar** (Bristol) on *Substrate and inhibitor interactions Class D OXA b-lactamases*.
9) **Jingxu Guo** (UCL) on *The X-ray structure of juvenile hormone dial kinase from the silk worm Bombyx mori*.
10) **Simone de Rose** (Exeter) on *Thermus thermophilus as a whole-cell factory for the production of extremolytes*.
11) **Alex MacPherson** (Bath) on *The allosteric modulation of C5 by knob domain peptides*.
12) **Jenn-Yeu Alvin Szeto** (Bristol) on *Characterising the structural and biophysical interactions between nonsense mediated mRNA decay factors UPF2, UPF3B and RNA*.
13) **Lainey Williamson** (Cardiff) on the *Crystal structure of Lysinibacillus sphaericus Tpp49Aa1 solved using serial femtosecond crystallography*.

The winners of the poster prizes were **Raul Cioaca**, **Alvin Szeto**, **Rachael Andrews**.

Mark Roe
University of Sussex

Elections to BCA Council

There will be elections this year for:

- BCA Vice President
- BCA Honorary Secretary
- Ordinary Member

Any two Members may make nominations, and such nominations should be accompanied by the written consent of the candidate to serve if elected. These must be received by the Secretary by 30th September 2021.

Remembering John Squire: His achievements and legacy

It was with great sadness that we learnt of the death of John Squire, Professor of Structural Biophysics in the University of London and Visiting Professor at Imperial College.

Professor John Michael Squire (B.Sc., Ph.D., C.Phys., F.Inst.P., C.Biol., F.S.B.) was internationally renowned for his research on the structural basis of muscle contraction. He joined Imperial College in 1972 where he established the Biopolymer Group within the Department of Metallurgy and Materials Science. He subsequently moved to the newly formed Biophysics Section in the Department of Physics in 1984, becoming a Reader and then Professor in 1995. In 1999 he became Head of the Biological Structure and Function Section within the newly established Division of Biomedical Sciences located in the Sir Alexander Fleming Building. After his official retirement in 2006 he maintained a strong and active interest in research through his ongoing affiliations with Imperial College and the University of Bristol, publishing his most recent paper in 2020.

John passed away on 31st January 2021, a victim of the deadly SARS-CoV-2 virus which has been causing havoc around the world since the start of 2020. John is survived by his wife, Melanie, their four daughters and ten grandchildren.

Over a research career of 51 years John established himself as a leader in the field of muscle research. Early in his career he introduced many of the key concepts in the field including the steric blocking model of thin filament regulation (with David Parry) and a general model for assembly of myosin filaments from the constituent myosin molecules (published in 1971, but only fully verified in recent years with the aid of new technology). Subsequently, using a combination of X-ray fibre diffraction and electron microscopy, he identified the particular structural features of bony fish muscle which make this an especially suitable system with which to observe the individual molecular steps by which muscles contract. Over a number of years, he proceeded to exploit this system to build up a detailed structural model of the mechanism of muscle contraction which he termed Muscle the Movie.

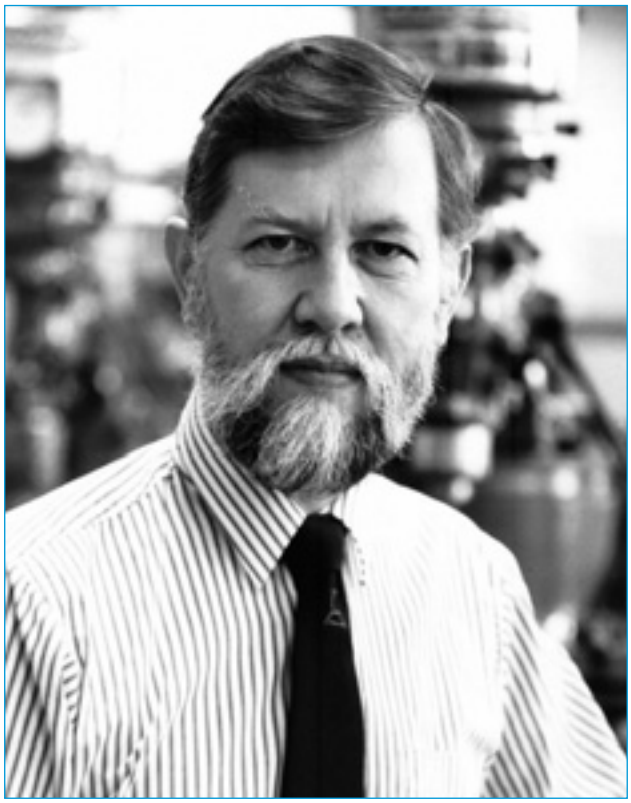
John's research on muscle contraction and related areas such as the blood vessel glycocalyx formed the basis of a substantial body of more than 250 publications. Alongside his primary research papers he also wrote many reviews and book chapters. Of particular note is his 700-page book: "The Structural Basis of Muscle Contraction", which was published in 1981 but still remains one of the best and most comprehensive introductions to the field.

John was also well known for his leadership within the scientific community. He founded and chaired the Collaborative Computational Project 13 (CCP13) which developed and supported software for the analysis of X-ray fibre diffraction data. He set up and organised scientific meetings including the Imperial Muscle Initiative meetings and, together with David Parry, a series of international workshops on Coiled-Coils, Collagen and Co-proteins which were held every 4 years in Alpbach, Austria. John was a member of the British Crystallography Association, and a member of the BCA Council and Editor of Crystallography News from1987 to 1995.

Throughout his time at Imperial College, John ran a thriving research group drawn from a wide range of nationalities and cultures. Within the group he fostered a supportive environment frequently leading to enduring friendships. The group and family members were regularly invited round to John and Melanie's house in Egham to a series of parties in their beautiful garden at which somehow the sun always seemed to shine. Many of his former students and postdocs who went on to build their own careers in science continued to work with him on collaborative projects. Additionally, he maintained a substantial network of collaborations with scientists all over the world. That so many were happy to continue to do science with John in this way serves as a testament both to the esteem in which he was held scientifically and to the fact that he was a pleasure to work with.

Ed Morris, Institute of Cancer Research
Pradeep Luther, Imperial College London

John Sinclair Reid 1942-2021



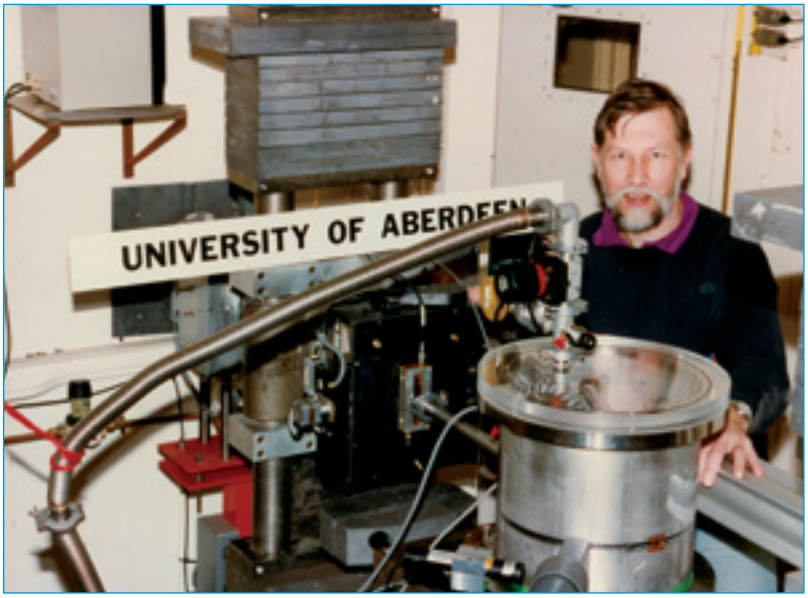
Crystallography was one of the many and varied subjects that John Reid taught at the Natural Philosophy (alias Physics) Department of the ancient University of Aberdeen. He was born in wartime Chorleywood (North London) in 1942, and after his early schooling, he was sent as a boarder to Robert Gordon's College, Aberdeen. Aberdeen was where he spent the rest of his life, graduating three times at the University and becoming, in turn, Assistant Lecturer, Lecturer and Senior Lecturer in Natural Philosophy. He had an unusual combination of degrees and an impressive collection of professional fellowships: B.Sc., M.Litt., Ph.D., F.R.A.S., F.R.Met.S., F.Inst.P., C.Phys. He had a keen interest in astronomy, meteorology and the history of physics, and he was a founder member of the Scientific Instrument Society. He was Curator of the Natural Philosophy Collection of Historic Scientific Instruments in Aberdeen. It was while demonstrating practical physics in one of the teaching laboratories that he met the undergraduate who later became his wife. Their joint interests in astronomy and navigation were useful practical skills in pursuing their love of sailing.

John's father had survived the World War I trenches of Belgium and France, and was later a business accountant, who loved carpentry. His mother had been a secretary. They lived in a house with plenty of books, which included volumes in French, German, Italian, Gaelic and Russian. It was aged 10 that he made his first valve radio and while at Robert Gordon's College, John made crystal sets (wireless receivers); he indulged in photography; and he constructed and flew model aircraft. He excelled at mathematics, science and geography. When his father retired from his London job, the whole family settled in Aberdeen. John became an active member of the Aberdeen Amateur Radio Society.
John's Ph.D. topic concerned the analysis of atomic motions in crystals derived from observations of diffuse X-ray scattering. This introduced him to a lifelong interest in diffuse scattering and the information that could be extracted from it. His initial calculations were performed in Algol 60 on an Elliott 803 computer, starting with the 1-phonon scattering in sodium chloride (NaCl). Later, he also used a triple-axis spectrometer at the PLUTO reactor at Harwell to study neutron scattering from huge sodium bromide (NaBr) crystals, which had been grown by 'Dai' Jones at Aberdeen. Together with Dr John Pirie and others, he developed the equipment necessary for a comprehensive study of energy-dispersive diffuse X-ray scattering using synchrotron radiation at the Daresbury Laboratory. For over 30 years he was a regular attendee at the triennial International Union of Crystallography Congresses. He published 16 papers in *Acta Crystallographica* and the *Journal of Applied Crystallography*, all related to diffuse scattering. His 1995 paper, "The analytical calculation of absorption in multifaceted crystals" has over 1000 citations (and counting!) on researchgate.net.

John retired from the University of Aberdeen in 2007, but continued his lifelong love of physics and the history of science. He continued to curate the nationally recognised Historical Scientific Instruments Collection at Marischal College, ran the Aberdeen Mechanical Society and was an active member of the Scientific Instruments Society (of which he had been a founder member, in 1983).

In his latter days, John bravely fought two cancers. He will be greatly missed by his family and friends; and by all those whom he taught at Aberdeen over a period of 50 years.

Moreton Moore
Royal Holloway University of London



***John Reid** with a home-built scattering chamber at station 7.6 at the Daresbury synchrotron source, November 1990.*

Meetings of interest

IN the continuing pandemic situation, many meetings are being cancelled or postponed. At the time of writing, all the meetings listed here were scheduled to go ahead either in-person or online, but there are likely to have been further changes since going to press. Further information may be obtained from the websites given. Assistance from the IUCr website is gratefully acknowledged.

Note that many online meetings charge little or no registration, so if there's a topic that's of particular interest but you'd rather not travel, you might check it out. Also, some meetings listed with a location may be running a mixed in-person/online format.

If you have news of any meetings to add to future lists, please send them to the Editor, **john.finney@ucl.ac.uk**.

8th Sep 2021 - 10th Sep 2021
Peptide-Membrane Interactions: Faraday Discussion
Online.
https://www.rsc.org/events/detail/37143/peptide-membrane-interactions-faraday-discussion

16th Sep 2021 - 17th Sep 2021
23rd Heart of Europe Bio-Crystallography Meeting (HEC23)
Online.
https://www.hec23.uni-bayreuth.de/en/index.html

19th Sep 2021 - 21st Sep 2021
78th Annual Pittsburgh Diffraction Conference
Online.
https://smb.slac.stanford.edu/news/PDC-2021/index.html

20th Sep 2021
4th Austrian Cryo-EM Symposium
Klosterneuburg, Austria.
https://ace.ist.ac.at/#section0

22nd Sep 2021
Grand Challenges in Quantitative Structure-Activity Relationships
Online.
https://www.euroqsar.org/

27th Sep 2021 - 1st Oct 2021
ICDD Rietveld Refinement and Indexing Clinic
Newtown Square, PA, U.S.A.
https://www.icdd.com/rietveld/

4th Oct 2021 - 8th Oct 2021
45th IUPAB Congress
Online.
http://iupab.org/iupab-next-congress/

11th Oct 2021 - 14th Oct 2021
International Conference on Materials Science and Engineering 2021
Brisbane, Australia, with online participation.
https://www.materialsconferenceaustralia.com/

15th Oct 2021 - 17th Oct 2021
10th International Conference of the Hellenic Crystallographic Association
Athens, Greece.
https://sites.google.com/view/hecra2020/home

31st Oct 2021 - 5th Nov 2021
Three Dimensional Electron Microscopy Gordon Research Conference
Newry, ME, U.S.A.
https://www.grc.org/three-dimensional-electron-microscopy-conference/2021

1st Nov 2021 - 5th Nov 2021
ICDD Clinic - Practical X-ray Fluorescence
Newtown Square, PA, U.S.A.
https://www.icdd.com/xrf/

15th Nov 2021 - 19th Nov 2021
African Light Source Conference
Online.
http://conference.africanlightsource.org/

16th Nov 2021 - 25th Nov 2021
ISIS Reflectivity Training Course
Online.
https://www.reflectometry.org/workshops/

6th Dec 2021 - 8th Dec 2021
Asia-Pacific Cryo-EM Symposium
Online.
https://www.apac-cryoem.org/

6th Dec 2021 - 17th Dec 2021
ICTP School on Synchrotron Light Sources and their Applications
Online.
http://indico.ictp.it/event/9645/

16th Dec 2021 - 17th Dec 2021
Italian Crystal Growth 2021 - Crystal Growth: from Theory to Application
Torino, Italy.
https://www.icg2020.net/

11th Jan 2022 - 14th Jan 2022
16th International Conference on Surface X-ray and Neutron Scattering (SXNS16)
Lund, Sweden.
https://www.sxns16.org

17th Jan 2022 - 22nd Jan 2022
Third Pan African Conference on Crystallography
Nairobi, Kenya.
https://pccr3africa.org/

28th Mar 2022 - 30th Mar 2022
Understanding Crystallisation: Faraday Discussion
York, U.K.
https://www.rsc.org/events/detail/41849/understanding-crystallisation-faraday-discussion

31st May 2022 - 3rd Jun 2022
17th European Powder Diffraction Conference – EPDIC17
Šibenik, Croatia.
https://www.epdic17.org/

9th Jun 2022 - 10th June 2022
Assembling Matter at all Scales
Dresden, Germany.
https://www.max-bergmann-symposium-2022.de/

19th Jun 2022 - 30th June 2022
Zürich School of Crystallography 2022: Bring Your Own Crystals
Zürich, Switzerland.
https://www.chem.uzh.ch/linden/zsc/index.html

10th Jul 2022 - 16th Jul 2022
16th International Conference on the Physics of Non-Crystalline Solids
Canterbury, U.K.
https://sgt.org/mpage/PNCS16

29th Jul 2022 - 3rd Aug 2022
72nd ACA Annual Meeting
Portland, OR, U.S.A.
https://www.amercrystalassn.org/future-meetings

21st Aug 2022 - 26th Aug 2022
CMD29 (Condensed Matter Division of the European Physical Society)
Manchester, U.K.
http://cmd29.iopconfs.org/Home

23rd Aug 2022 - 27th Aug 2022
Thirty Third European Crystallographic Meeting (ECM33)
Versailles, France.
https://www.ecm33.fr/

11th Sep 2022 -16th Sep 2022
15th Biennial Conference on High Resolution X-Ray Diffraction and Imaging (XTOP 2020)
Minsk, Belarus.
https://www.xtop2020.atomicus.by/

26th Sep 2022 - 30th Sep 2022
Integrative Data-Intensive Approaches to Drug Design
Heidelberg, Germany.
https://www.euroqsar2022.org/

Endpiece: The first anthropogenic quasicrystal?

THE mention of quasicrystals and generalised crystallography on page 4 reminded me of a particularly interesting (to me!) paper in the June 2021 issue of *PNAS*[1]. While I may not wish to remember what happened on 16th July 1945 (the Trinity test – the detonation of the first plutonium atomic bomb), this paper discovered that one of the outcomes of the test was the formation of a quasicrystal within the trinitite glass formed by the explosion (figure 1). Thus it appears that a quasicrystal (see figure 2) was made (admittedly unintended) by man some four decades before they were first realised in the laboratory[2]. Not only is this discovery of interest in demonstrating that quasicrystals can be made in high-temperature, short-duration shock events (in that test estimated at about 1,500C and pressures up to 5 to 8GPa[1]), but also the phase itself (of composition $Si_{61}Cu_{30}Ca_7Fe_2$) is unique: no other known mixtures of Si, Cu and Ca have been shown to be quasicrystalline, nor is there any other known quasicrystal in which the dominant element is Si.

Figure 1: The red trinitite sample in which a novel quasicrystal was found (reproduced under licence from reference 1).

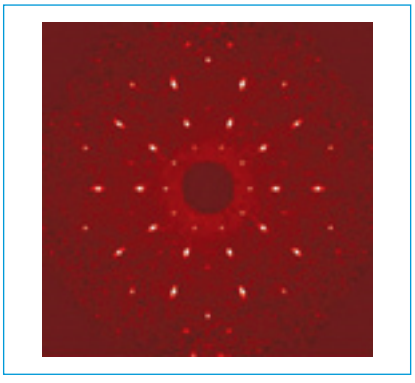


Figure 2: X-ray diffraction pattern along the fivefold axis on the quasicrystalline fragment (reproduced under licence from reference 1).

Interestingly, the Trinity test conditions were similar to those created by the impact of the Khatyrka meteorite impact which also produced quasicrystals. And as that event is thought to have occurred about 4.5 billion years ago, those quasicrystals are probably about as old as the solar system! Apart from these results suggesting conditions that might be used for further searches for quasicrystals, one might also look at things the other way round. If and when other naturally-formed quasicrystals, are found, we might reasonably suggest that such extreme temperature-pressure conditions caused their formation. Perhaps relevant to the detection of undeclared locations where atomic bombs may have been tested?

John Finney
UCL

References:

1. L. Bindi *et al. PNAS* **118** (22), e2101350118 (2021). https://doi.org/10.1073/pnas.2101350118.
2. D. Schechtman *et al. Phys. Rev. Lett.* **53**, 1954 (1984).

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