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President's Letter – Spring 2024

Santiago García-Granda

As the year goes on, the IUCr continues building the future, trying to be attractive for the new generations and engaged in the scientific solutions to face the global problems and contribute to maintain and improve the live conditions in the planet, being instrument of peace, freedom and respect for the environment.

In this first letter of 2024 I would like to send a message of hope for the future of our Union. We have been praising our glittering past on the occasion of the 75th anniversary of our first General Assembly, the 26th in the triennial series, in Melbourne. It is important to recognise, learn from and even imitate the pioneers, but perhaps it is just as important to look to the future through the new generations, in the same way that scientific objectives have evolved from classical crystallography to all aspects of structural science, as the banner of our next Congress and General Assembly, IUCr27 in Calgary in August 2026, highlights: 'Embracing Structural Science'. New times call for new ways and new people, and generational change is the key factor in any organisation that intends to endure. That is why the IUCr needs to put its efforts in offering leadership opportunities to young people and integrating all structural scientists in a transversal way in our plans of scientific cooperation with the widest possible transversality.

One of the aspects that should differentiate our renewal, in the current social context, is the incorporation of female leadership in a natural way in our activity.

A second aspect is the identification of the IUCr as a global scientific organisation, with local representation through the Regional Associations and National Committees, which must have the capacity to operate with broad autonomy, but which must have a clear identification with the global parent IUCr. At the moment our five Regional Associations cover in a very reasonable and convenient way the five continents. It is important that all of them participate in a rational way in the leadership of the IUCr and that they strengthen the links of collaboration between them.

On the other hand, the 55 National Committees, which make up the General Assembly, should also, both through their Regional Associations and through their representation in the IUCr, make their voice heard, participate actively in the IUCr's activity and establish multinational collaborations. One of the objectives of the Executive Committee is to extend this number to the countries where Crystallography and Structural Science is developing so that they can contribute to enrich the IUCr with their inputs.

The aim is to create a more cohesive image of the IUCr and also to take advantage of the capacity of the Regional Associations and the National Committees to raise awareness of the IUCr. In particular, iIt is important to show through the social media a coherent and close image to society from a scientific analysis of the main challenges we face as a global society, and the specific effects in a community or nation or in a given geographical area.

The sustainability of resources for life on the planet - in all its diversity - is a key issue that humanity is not satisfactorily resolving. The International Year of Basic Sciences for Sustainable Development 2022/2023 has provided a new look at sustainability from a scientific point of view, and managed to capture the attention of the highest global institutions, as the United Nations, UNESCO or ISC and especially, gave a voice to the new generation of scientists to address the problems and provide sustainable solutions.

The natural follow-up to the success of the International Year of Basic Sciences for Sustainable Development, IYBSSD, is the International Decade of Sciences for Sustainable Development, IDSSD, which was launched by the United Nations on 25 August 2023 and will run until 2033.

The broad period of the Decade, beyond 2030, will allow to assess progress and modulate the SDGs (Sustainable Development Goals) with the tools of basic science and to join efforts to train new generations of scientists increasingly concerned with solving global problems, in a cross-cutting and cooperative way and giving women scientist the chance to be protagonist, contributing to and lead the paradigm shift.

Structural scientists, can apply their developments to environmental remediation and recovery as well as to the optimal reuse of resources or the production of clean energy and solve global environmental problems by seeking an optimal distribution of the planet's limited resources.

The exploration of other off-planet resources is another avenue in which the experience and knowledge of structural scientists will be extremely valuable. These people should be ready to be fully involved in changing the priorities and the way of live of the humanity in the following decades.

In early March, after the EC bymonthly meeting, the Journal Management Board will meet in Chester on 7 and 8 March, and on 11 and 12 March, the spring meeting of the Finance Committee will take place in Lund, Sweden.

At both meetings important decisions will be taken about the most important area of activity of our Union, our 10 journals, which, as we all know, is undergoing major changes due to the influence of new forms of publishing and the emergence of new practices of publishing business. In this regard, the executive committee, in conection with the Editor-in-Chief and the Executive Managing Editor, is devising new ways to revitalise our publications, with initiatives such as the setting up of an independent working group to provide a vision for the future development of our publishing activity in the new environment.

In parallel, the finance committee will analyse the impact of the publishing section on the Union's finances and what initiatives can be implemented to strengthen the Union's funds.

As announced, the ISC will vote for the new statutes on February 29th and, after the initial fears and an unanimous action by the scientific unions, the position of the unions, and the IUCr among them, maintains its full capacity for scientific initiative and influence at the global level and in the decisions of the International Science Council. Meetings with the ISC President, the 28th of February, will be atended by Hanna Dabkowska and myself.

The Chester's office is doing its job as professionally as ever, with the only change of the incorporation of Kezia Bowman, who joined in January as a Marketing Executive and is already doing also a fantastic job settling into the role, as progress is being made for the implementation of the Customer Relationship Manager (CRM) and new website. On the other hand, we have received the Purpose Vision and Values and we had over 274 responses. The next steps will be for the EC finalise the Purpose and Vision and Values statements. Once we have these, the IUCr CEO will draft a Mission statement that covers all the important issues on what IUCr will do to achieve its Vision and Purpose for the EC to approve, before we circulate to members. Furthermore, one memoradum of understanding has been formalizaed with the OIC Ministerial Standing Committee for Scientific and Technological Cooperation, ‘COMSTECH’, as a framework of cooperation.

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

Thanks to IUCr Newsletter Editor Mike Glazer, his team and all contributors for making possible, as every quarter, a new quarterly issue and for continuing to be the communication reference for our community.

Many thanks to all for for contributing to sustain and reinvent the IUCr from anywhere in the world.

All the best!

Editorial

Mike Glazer

SrTiO3: Mesmerising picture of a low-frequency distortion mode for a wave-vector at the R-point of the cubic Brillouin zone (Crystalmaker11: Phonons Explorer)

Spring is here in the UK at last! I am always glad when winter is on its way out. I have just returned from a two-day Finance Committee in the city of Lund (Sweden), where I heard about the creative work carried out by our new Marketing Executive, Kezia Bowman. Kezia will be involved in developing marketing strategies to promote the IUCr and its publications and initiatives, and creating engaging content for diverse audiences. I wish her success in this important role.

In this issue of the Newsletter, we have two articles from the Hargittais , one on the Russian crystallographer Vladimir A. Koptsik, who was an important contributor to symmetry groups, especially the so-called Shubnikov groups. These groups, sometimes called colour groups, explore all the possible symmetry operations in which alternating colours (say black and red) can be included. Most crystallographers will already be familiar with the 230 space groups, which relate possible atomic positions subject to symmetry constraints in three dimensions. The Shubnikov groups, add the possibility of positions for species with alternating properties, such as those like up and down electron spins. This is important for the study of magnetic crystal structures. There are 1651 such groups, and these were tabulated and illustrated by Koptsik in a weighty book (Шубниковские группы: 1966 Moscow University). I actually have a copy in front of me and I have to admire the enormous body of work that Koptsik achieved.

The other Hargittai article is on Johannes Kepler, he of planetary fame. While his work on planetary orbits is well known, he was also interested in crystals and why they formed such symmetric shapes. Why, for example, were snow flakes hexagonal in shape? In 1611, he conjectured that there must be some underlying regularity in their internal structure, though he could not know what this structure actually was. He, along with others, such as Robert Hooke, considered the close packing of spheres as a way of explaining the external morphology of crystals: today we know that it is periodic arrangements of atoms and molecules that are responsible for the external shapes of crystals. Kepler famously considered, for instance, the three-dimensional packing of spheres (this was related to the problem of how to keep cannon balls from rolling around the deck of a warship). Kepler's conjecture was that the so-called cubic and hexagonal close packings were the most stable arrangement (think of the way oranges can be stacked together on a fruit stall). Surprisingly, his conjecture was not fully proved until very recently by Hales T, Adams S M, Bauer G, et al. (A Formal Proof of the Kepler Conjecture. Forum of Mathematics, Pi. 2017;5:e2. doi:10.1017/fmp.2017.1). So that took just over 400 years to solve!

I was intrigued when a friend of mine in India sent me a poem (ref) that she had found that mentioned a famous scientist who played an important role in our understanding of x-rays and atomic physics, namely Harry Moseley. He was killed in battle at Gallipoli in 1915 and this poem was published 10 years after. Many years ago, I went into the office of one of our secretaries and noticed a cardboard box in the corner behind the door. I also saw that every time someone entered the room, the door was slammed against the box. I looked inside the box, and there was one of Moseley's original X-ray tubes, very similar to the one seen being held by Moseley in the image at the beginning of this article. Miraculously, despite its fragility, it had survived despite its rough treatment. It can now be seen in the small museum at the Clarendon Laboratory.

One of Moseley's x-ray tubes found in the Clarendon Laboratory, Oxford

JOHANNES KEPLER – THE FIRST SCIENTIFIC CRYSTALLOGRAPHER

Istvan Hargittai and Magdolna Hargittai

Budapest University of Technology and Economics

Johannes Kepler's (1571−1630) best-known contribution to science is his three laws of planetary motion. He was a pioneer in model building, which he extended into the third dimension, though his famous planetary model proved to be a non-discovery. He discussed the stacking of equal spheres when examining snowflakes and advanced the notion that internal structure determines the external shape. This was relevant to a fundamental issue in crystallography, and he has been considered the first scientific crystallographer.

Johannes Kepler, line engraving by N. Dietz (Wellcome Collection)

Science has made great use of Kepler's works over the centuries, but Kepler the man himself has been little known. Galileo did not give him much recognition, and Newton did not mention him in most parts of his Principia or did so only in passing [1]. Kepler's principal languages were German and Latin, and his penetration into English literature was slow. Then, in the 19th century, two monographs in English were devoted to Kepler [2, 3]. The first complete biography of Kepler was published in German by the great Keplerian scholar Max Caspar and translated into English in 1959 [4]. Arthur Koestler's monumental book, The Sleepwalkers, appeared also in 1959 [5]. Part of it is a biography of Johannes Kepler, which was also published separately as a little volume, entitled The Watershed [6]. These publications broke the ice and did a great deal to make Kepler better known. Since then, there has been a growing amount of literature about Kepler.

Kepler's three laws of planetary motion have earned him a solid place in the domains of physics and astronomy. Just as a reminder: 1 The orbit of a planet is an ellipse, with the Sun at one focus. 2 The line joining a planet to the Sun sweeps out equal areas in equal times. 3 The squares of the periods of the planets are proportional to the cubes of their mean distances from the Sun.

Kepler's work relevant to crystallography is documented in the Historic Atlas of Crystallography [7] and more extensively in our volume about the role of symmetry in scientific discoveries, giving emphasis to model building [8].

Closely packed spheres by Kepler [9]

Kepler's treatise, De Nive Sexangula (The Six-cornered Snowflake), was published in 1611 in Latin [9], followed by an English translation 355 years later.

The cover of De Nive Sexangula and J. M. Wacker von Wackenfels' portrait by Aegidius Sadeler in the Scientific Library of the City of Trier (in the public domain, File:Johann Matthäus Wacker von Wackenfels.jpg - Wikimedia Commons)

Kepler wrote this 24-page treatise as a New Year's gift to his patron, J. M. Wacker von Wackenfels (1550−1619), thereby making his name immortal in science history. Wacker von Wackenfels was a scholar and author interested in philosophy and history. He originated from modest circumstances and worked himself up the societal ladder through scholarship, hard work, and advantageous marriages. He received support for his studies, earned hereditary nobility, and a position in the high court of the Holy Roman Empire.

Kepler was the first credited with discussing the problem of packing equal spheres. In this work, he discussed the structure of the honeycomb, and when trying to figure out why the snowflakes have hexagonal shapes, he considered the question in three dimensions. This contrasts with Descartes, who, when discussing snowflakes a quarter of a century later, considered them only in the plane [10].

In De Nive Sexangula [9], Kepler realized that external shape is correlated with internal structure. The external polyhedral shape grows naturally because of the internal regular arrangements of the building elements. In contrast, a symmetrical polyhedral shape does not necessarily mean an ordered internal structure. This is obvious today, yet even some widely used introductory chemistry texts state that crystals and amorphous bodies differ in their shapes: it is easy to cut a piece of glass to look perfect, but it will still remain amorphous.

Alan L. Mackay called our attention to the importance of this knowledge for the courtesans in sixth-century India, according to the Kama Sutra by Vatsyayana. They had to learn mineralogy as they were often paid in precious stones. They had to be able to distinguish genuine crystals from paste [11]

Kepler felt the excitement of discovery when looking at snowflakes in cold, dry weather. They all were hexagonal in their full shape and symmetry, but they came in a great variety, and no two looked the same. As he was considering the origin of these perfect shapes, he concluded that the uniform arrangement of their elemental building particles must be the reason for these shapes. These building particles were water molecules, but of course, he could not know this. However, he correctly assigned the formation of shapes to very dense internal packing. Furthermore, he correctly described cubic closest packing and hexagonal, and simple cubic packing. He could not explain why the snowflakes have sixfold symmetry but conjectured that hexagonal packing would provide the maximal close packing. Thomas C. Hales referred to Kepler's conjecture as: "No packing of congruent balls in Euclidean three-space has a density greater than that of the face-centered cubic packing" [12]. Hales published his proof of Kepler's conjecture in 2005 in the Annals of Mathematics and dedicated his work to the memory of the Hungarian geometer László Fejes Tóth.

Statue of Sir Walter Raleigh by William McMillan in Greenwich (photograph by the Hargittais) [13] and portrait of Thomas Harriot, 1602, by an unidentified painter from the collection of the University of Oxford (in the public domain, File:ThomasHarriot.jpg - Wikimedia Commons)

Kepler's discovery is considered a foundation of modern crystallography, though he may not have been the first to recognize how the densest packing of congruent spheres is accomplished. As often happens in science, there was another person, Thomas Harriot (c.1560−1621), who in England, in 1599, came up with a similar observation of the arrangement of densest packing. He was an astronomer, mathematician, ethnographer; he improved navigational techniques and created advanced maps and participated in expeditions. He was the scientific advisor for one of Sir Walter Raleigh's (1552or4−1618) expeditions around 1587. Raleigh posed Harriot the question about the most economical means of storing cannon balls in his ship. This was thus a question about the densest packing of equal-size spheres. Both the question poser and the one who responded deserve our note. Harriot corresponded with Kepler about optics, but there is no information on whether their exchange contained any reference to densest packing.

Keper's treatise inspired Alan L. Mackay to respond in 1981, 370 later, with his paper "De nive quinquangular" [14]. Mackay predicted what then was to be called "quasicrystals." For a beautiful computer-automated drawing of a "Pentagonal snow crystal" by Robert H. Mackay in 1975, see [15]. Philip Ball celebrated the fourth centenary of Kepler's publication about the six-cornered snowflake with an essay in Nature [16]. There as, elsewhere (see, eg, [17, 18], are presented the attempts over centuries to understand and explain the hexagonal shapes of snowflakes. I.I. Shafranovskii called attention to Kepler's attempt to create a pattern of fivefold symmetry [19].

Kepler's Planetary Model based on regular solids [20], and a Hungarian postage stamp with Kepler's portrait and his model

Kepler graduated as a theologian, but his first position, at the age of 20, was as a teacher of mathematics and astronomy in Graz, Austria. He was unhappy with this job and found an escape in thinking about Copernicus' new ideas concerning the solar system, the six planets, and their distances from the Sun. Then, while drawing some figures on the blackboard, a new idea suddenly came to his mind. It was like a lightning bolt, and he was so shaken that he noted the date when this happened: July 9, 1595. The idea never left him for his entire life. He started with a large circle with a triangle in it and another circle within the triangle. He suddenly realized that the ratio of the two circles was the same as that of the orbits of Saturn and Jupiter, the two outermost planets. He continued inscribing into the next interval between Jupiter and Mars a square, between Mars and Earth a pentagon, and between Earth and Venus a hexagon. He calculated the ratios of the radii of the subsequent circles and compared them with the results of Copernicus. He was soon disappointed because they did not match. At that point came yet another lightning bolt, the realization that he should expand his considerations into the third dimension, just as the planets exist in three dimensions, in space rather than merely on the plane. So, he used spheres rather than circles and polyhedra rather than polygons.

The five regular polyhedra of Plato were the perfect solution, matching the six planets that were known at the time. Except for the orbits of Saturn and Mercury, his results mostly agreed with those of Copernicus. To eliminate the discrepancies, he gave some thickness to his orbits, and this approach improved the agreement. This is also how he arrived at the great discovery of the elliptical orbits of the planets. Kepler wrote a small book, Mysterium Cosmographicum [20]. This was in 1597, when he was 26 years old. This book already contains the seeds of all of Kepler's later discoveries. It also shows him as a modern scientist who knew that his model could be right only if it were consistent with observation. It was in this connection that he introduced the concept of observational error. Later in his life, when he realized that his model still had problems, he extended his considerations to general harmonies. He augmented his geometrical model with the principles of harmony. By doing this, he returned to ancient notions, which was a retreat, but he had no other recourse, as at the time, there was no other recourse. Kepler expressed the complementary nature of geometry and harmony in his Harmonices Mundi (1619) [21].

Kepler's planetary model was an incorrect model. Some considered it childish. Others recognized its fertility for a host of other scientific endeavors. This was not a unique case in science history when an incorrect model paved the way to correct results. Aaron Klug quoted the philosopher A. N. Whitehead, who coauthored Principia Mathematica with Bertrand Russell: "It is more important that an idea be fruitful than that it be correct." When Klug compiled his Nobel lecture for publication, he included a picture representing his original idea of nucleation, which turned out to be erroneous. Klug wanted to include it because it showed how science was a process of establishing the truth (emphasis by Klug) [22]. Klug's notion reflected what Kepler himself noted: "The roads by which men arrive at their insights into celestial matters seem to me as worthy of wonder as those matters in themselves" [23].

In conclusion, let us quote Koestler concerning this matter: "That some of his answers were not right does not matter. As in the case of Ionian philosophers of the heroic age, the philosophers of the Renaissance were perhaps more remarkable for the revolutionary nature of the questions they asked than for the answers they proposed. Paracelsus and Bruno, Gilbert and Tycho, Kepler and Galileo formulated some answers that are still valid; but first and foremost, they were giant question masters. Post factum, however, it is always difficult to appreciate the originality and imagination it required to ask a question which had not been asked before. In this respect, too, Kepler holds the record" ([6], p. 61).

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Recent news from the European Crystallographic Association

Arie van der Lee

European crystallographers usually hold their Crystallographic Meeting (ECM) in Europe in years when the International Union for Crystallography does not organize its triennial congress. 2023 was such a year without an ECM when the worldwide crystallographic community, including Europe, gathered in Melbourne, Australia. The ECA Council meeting was held remotely in two different sessions to ensure as high an attendance as possible, on the 20th and 22nd of September 2023. Meetings of the Executive Committee were organized remotely just before the Council Meeting on the 11th and 12th of September 2023 and another one in Poznań, Poland, from the 2nd to the 4th of February 2024.

A considerable part of the business at the ECA Council Meetings naturally concerns the planning of future European Crystallographic Meetings and Schools, and Councillors receive progress updates on the planning of upcoming meetings as well as the opportunity to vote for the location of future ECMs and ECSs. Due to the ongoing conflict in Ukraine, where ECM35 was due to be held in 2025, a proposal was made by the Polish

Crystallographic Association in collaboration with ECM35 organisers and other Ukrainian colleagues to move the location of the conference to Poznań, which the Council approved. A bid from Czech colleagues to hold ECM36 in Prague (at the same location as the 25th IUCr Congress in 2021) was also presented and approved.

The Prizes awarded by the ECA were also discussed in detail. The oldest Prize is the Max Perutz Prize, which is awarded in recognition of meritorious achievements in any branch of crystallography, and the Erwin Félix Lewy Bertaut Prize, which is awarded jointly with the European Neutron Scattering Association to a young scientist in recognition of notable experimental, methodological, or theoretical contributions to the investigation of matter using crystallographic or neutron scattering methods). The Alajos Kálmán Prize was created more recently and is awarded jointly with the Hungarian Chemical Society in recognition of outstanding scientific contributions in the field of structural sciences. At the Council meeting in September, proposals were heard and approved for the incorporation of two new prizes related to ECA: the George M. Sheldrick Prize (awarded to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences) and the Lodovico Riva de Sanseverino Prize (awarded in recognition of notable contributions to the dissemination of crystallography in the field of education at all levels). More information is available online: https://ecanews.org/prizes/. All five prizes will be awarded this year at ECM34 in Padova in August.

Group photo of ECS8 held in Berlin (June 2023). Photo by Manfred Weiss.

Finally, of interest to younger members of the crystallographic community, the ECA Council heard the report on the 8th European Crystallographic School (ECS8), which took place in person in Berlin, Germany, in June this year. European Crystallographic Schools combine lectures and hands-on tutorials to provide attendees with a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater to a broad range of interests. ECS9 will take place in 2024 in Nancy, France, and a successful bid takes ECS10 to Ohrid, North Macedonia, in 2025. For further information on the ECS, please visit https://ecanews.org/european-crystallography-school/.

Early February 2024, the ECA's Executive Committee had the chance to visit the Poznań Congress Center, where ECM35 is envisioned to be held, and to speak, not only with the main local organizers Grygoriy Dmytriv and Maciej Kubicki, but also with people from Adam Mickiewicz University (AMU), the Professional Congress Organisation (AMU Foundation), and the Poznań Convention Bureau.

The ECA finances were discussed extensively: it was decided to increase the part of the budget allocated to support schools, workshops, and congresses, in particular for the ECA's own European Crystallographic Schools.

The ECA's General Interest Group 3 (GIG-03: Education in Crystallography) received a grant from the Royal Society of Chemistry (£5k), for the preparation and dissemination of a series of ten video interviews to celebrate the importance of women in the field of crystallography and science, while, at the same time, raising awareness about the pitfalls and obstacles on the way to reach gender parity in science. The first video will be launched in June 2024. GIG-03 is also preparing a Crystallography Video Competition (using a grant obtained from the Cambridge Crystallographic Data Centre) for schools in different European countries. The aim is to present the winning videos at the next European Crystallographic Meeting in Padova in August 2024.

European crystallographers continue to meet during the ECA's monthly lunchtime webinars, a successful series of online seminars covering all sub-disciplines in crystallography and organized by the ECA's young crystallographers. Eight lunchtime webinars took place from April 2023 until March 2024. Another series of webinars, the Distinguished Lectures on Quantum Crystallography and Complementary Fields, initiated by the ECA's Special Interest Group 2 (Quantum Crystallography) and the IUCr Commission on Quantum Crystallography continued as well: eight webinars took place, usually with two lectures during the same webinar.

80th Annual Pittsburgh Diffraction Conference

Simone Brixius-Anderko, Uta Ruett and Matthias Zeller

The 80th Annual Pittsburgh Diffraction Conference took place from October 15th to 17th, 2023, at the Wyndham Hotel situated on Pittsburgh's Oakland Campus. Nestled amidst the University of Pittsburgh and Carnegie Mellon University, Schenley Park, Phipps Conservatory and Botanical Gardens and the Carnegie Museums of Art and Natural History, this location provided an excellent setting for this event.

The Pittsburgh Diffraction Society (PDS) is a non-profit organization dedicated to advancing fundamental and applied diffraction and crystallographic research and to fostering the exchange of ideas and information. The PDS was founded by Surain S. Sidhu, who organized the first Pittsburgh Diffraction Conference at the University of Pittsburgh eighty years ago in 1943.

The 2023 conference was attended by 127 registered participants and featured 48 oral presentations and 20 poster presentations in sessions focused on all areas of diffraction, from applied science to protein crystallography. The conference was chaired by Simone Brixius-Anderko (University of Pittsburgh), who was supported by a team of over 16 organizers and session chairs from all over the country.

Preceding the main conference, a workshop on Phenix, which is a comprehensive software package for macromolecular structure determination, gathered 20 attendees led by the experts Dorothee Liebschner (LBNL), Tom Terwilliger (New Mexico Consortium), Pavel Afonine (LBNL) and Christopher Williams (Duke University).

The conference commenced with an opening reception on October 15th, followed by keynote lectures delivered by two former PDS' Sidhu Award winners, which is given to outstanding scientists within six years after earning the Ph.D. or equivalent. Erica Ollmann Saphire (the 2003 Sidhu awardee, now the head of the La Jolla Institute for Immunology) presented on the role of diffraction and Cryo-EM in fighting diseases in her talk "Antibodies against Emerging Infections: A Global Collaboration". Chong-Yu Ruan, awarded the Sidhu price in 2005, reviewed recent developments in ultrafast electron diffraction in his talk on "Femtosecond electron crystallography and microscopy: recent advances and applications". The keynote lectures were followed by a Young Investigator Platform that gave the upcoming researchers Tyra Douglas (ANL), Jordan Kelly (Duquesne), Vanessa Moresco (UC Riverside), Ari Selzer (Pitt), Sylwia Pawledzio (ORNL) and Giancarlo Gonzalez-Areizaga (Pitt) selected from student and postdoc poster submissions to present their projects and findings in short presentations.

In the spirit of the 80th jubilee of the Pittsburgh Diffraction Conference were the closing sessions of the 1st day, provided by William Furey (Pitt) and John P. Rose (University of Georgia) with recollections from 46 years of Pittsburgh Diffraction Conferences opening the birthday party, reception, and cake, which was generously sponsored by Rigaku. The following Karaoke session brought out sides of people very few expected.

October 16th started with a keynote session presented by Andrew Kruse of Harvard ("Structural basis for antibody fragment modulation of a G protein-coupled receptor"), after which the conference continued with two parallel sessions covering both physical and life sciences (aka "structural biology"). The structural biology section featured sessions on "Structure-based drug design", "Synergy of Computation and Crystallography for Structural Biology" and "Crystallography meets CryoEM". The Physical Sciences sessions covered "Latest developments at light sources", "Spins, phonons, and disordered states in complex materials" and "Investigating Materials' Structures and Properties using X-ray Diffraction Microscopy". Short presentations by vendors and sponsors and poster sessions and presentations complemented the sessions, and the day was ended with the traditional Banquet Dinner and some fun activities.

A keynote lecture by Daniel Shoemaker (UIUC) titled "Inorganic quantum crystallography: Discovering materials in the computer and in the lab "started sessions on the 17th, followed again by parallel sessions covering "Structure-property relationships in Quantum and Layered Materials" and "Materials under High Pressure – Using Diffraction Techniques to understand Synthesis Pathways, Phase Transitions and Phase Behaviors" for the Physical Sciences, and "High Pressure in Macromolecular Crystallography" and "General

Interest and cool techniques" on the bio-side of crystallography. Short vendor presentations and more opportunities to meet at posters and talk to vendors enabled inspiring discussions. Cora Lind-Kovacs delivered a presentation on behalf of the American Association to Advance Powder Diffraction (AAAPD), outlining preliminary results that compared worldwide high-resolution powder diffraction at user facilities. The presentation raised concerns regarding the competitiveness of the user facilities within the United States.

The meeting was concluded by the Society's business meeting. The Chung Soo Yoo poster awards, established by the PDS in his honor, were presented to the graduate students presenting the best posters at the conference. These were presented to Michael P. Dalton (Stony Brook University, NY) and Jordan Kelly (Duquesne University, Pittsburgh). Simone Brixius Anderko gave a summary of the conference and announced the winners of the vendor raffle, and Matthias Zeller gave an overview of the Society's finances in the Treasurer's report. Elections for positions on the PDS board were announced, and candidates for the offices of Treasurer and secretary, as well as for chair-elect for 2025 were asked to come forward. The president of the PDS, Uta Ruett (ANL), asked for nominations for next year's Sidhu Award and for future hosts for the upcoming conferences. The business meeting was closed by next President-elect Jeney Wierman, inviting to next year's Annual Pittsburgh Diffraction Conference at CHESS on the Cornell campus, in upstate New York, in October 2024. Please see the PDS website for upcoming details.

We would like to thank all our sponsors and exhibitors: University of Pittsburgh School of Pharmacy, Argonne National Laboratory, MiTeGen, Art Robbins Instruments, Formulatrix, Crystal Positioning Systems, Rigaku Americas, Dectris, Anton Paar and STP Labtech, without whose support the conference would not have been possible. A special thank also goes to Burroughs Wellcome Fund, which granted generously a proposal sent in by Denise Okafor (Penn State University) requesting travel support for selected attending students, postdocs and early career scientists, by granting a proposal sent in by for the PDC 2023.

Figure 1 William Furey (Pitt, right) and John P. Rose (University of Georgia, left), who gave the two presentations on the history of the PDC, with the 80th anniversary birthday cake.

Figure 2 The karaoke session. From left to right: James Weng (ANL), Alexis Paskach (U. Alabama Huntsville), Tyra Douglas (ANL), Stephany Webb (PITT). In the front (back to audience) is Cora Lind-Kovacs (Toledo) taking a break from “singing”.

Figure 3 Eric Reinheimer and Joe Ferrara (both from Rigaku), also with 80th anniversary birthday cake (which Rigaku sponsored).

A curious poem

Mike Glazer

Recently, a friend of mine in India came across a strange poem originally published in the Journal of Chemical Education in 1925, having noted that it seemed to have some relevance to crystals and, in particular, to the name Moseley. This immediately struck me as interesting, especially since Moseley's name has a special connection with Trinity College at the University of Oxford and the Clarendon Laboratory. So who was this chap, Moseley?

Well, he was Henry Gwyn Jeffreys Moseley, known usually as Harry Moseley. And his claim to fame, especially in the field of Crystallography, was indeed profound. He graduated from Oxford in 1910, spent some time in Manchester with Ernest Rutherford, and then returned to Oxford to carry out his research in 1913.

Now, it is important to recall that at the beginning of the 20th century, one of the outstanding questions that needed settling had to do with the nature of X-rays (originally discovered in 1895 by Wilhelm Roentgen). The burning question for physicists then was: are X-rays particles, or are they waves? Most scientists believed the wave theory, but some, including William Henry Bragg (WHB), thought they consisted of neutral particles. Then, in April 1912, an important experiment was carried out at the suggestion of Max Laue, a Privatdozent at the Institute of Theoretical Physics in Munich, but without the agreement of Arnold Sommerfeld, the head of the institute. The actual experiment was carried out in secret one night by Walter Friedrich, an assistant of

Sommerfeld (see https://www.iucr.org/news/newsletter/volume-28/number-3/walter-friedrich-unplugged-his-1963-interview-in-east-berlin) and Paul Knipping, a student of Sommerfeld. The experiment consisted of shining a beam of X-rays onto a crystal and then recording the scattering of the X-rays on photographic film. After several failed attempts, they finally obtained photographs that indicated that the X-rays were deviated by the crystal and even formed sharp spots on the film. This seemed to demonstrate that the X-rays had been diffracted by the atoms in the crystal, thus proving that X-rays were wave-like. Laue, later ennobled as von Laue, received the Nobel Prize in Physics in 1914. Although Friedrich and Knipping did not share the prize, Laue divided up the prize money between them. You can read Laue's amusing account of the experiment at https://www.iucr.org/news/newsletter/volume-27/number-1/address-by-professor-von-laue-before-the-first-iucr-congress-in-1948.

In the summer of 1912, word of this important experiment reached William Henry Bragg (WHB), then Professor of Physics at the University of Leeds. He then set about trying to show that he could explain the effect with his particle theory. His son, William Lawrence Bragg (WLB), had just graduated from Cambridge University, and he joined his father in conducting experiments to demonstrate the viability of the particle theory. The experiments all failed, but in August that year, WLB, while back in Cambridge, suddenly realised that Laue's results actually supported wave theory rather than his father's corpuscular theory. WLB's theory was remarkably simple since it drew upon well-known theories of the reflection and scattering of light.

WLB's 1912 notebook showing the first statement (near the top) of the later called Bragg's law (courtesy of the Royal Institution),

From this, WLB produced the equation that later, after modification, became known today as Bragg's Law. This took the form of a cosine function, where the angle q referred to the angle of incidence of X-rays on planes of atoms in the crystal. In this formula, l is the X-ray wavelength and d the distance between the planes. Whenever this equation was satisfied for all three terms, l, d and q simultaneously, the scattered X-ray left a spot on the film. WLB was able to show that it was possible to use this to derive information about the structures of crystals and that he could explain all the spots seen on the Laue diagrams as arising from diffracted X-rays with different wavelengths and from different planes within the crystal. He wrote a paper on this discovery that was read by J.J. Thomson on 11 November 1912 at the Cambridge Philosophical Society. Following this, he worked closely with his father to show how to solve crystal structures in numerous materials throughout 1913 and 1914 until all research was interrupted by the First World War. In 1913, WLB made use both of Laue's film method and also WHB's recently developed ionization spectrometer. The spectrometer gave more precise measurements than the film method (by the way, WHB's ionization spectrometer can be seen as the forerunner of the automatic diffractometers universally used today in crystallographic research). I suggest that it was the use of WHB's spectrometer that led in 1913 to changing Bragg's formula to the more familiar sinusoidal function that we use now

This is because it is more natural when using a spectrometer to measure angles from the incident beam direction, thus 90 degrees minus WLB's original angle q. Both father and son shared the 1915 Nobel Prize in Physics during the war.

Letter from Moseley to his mother 4 November 1912

WHB was present at the talk and afterward told Harry that his son, WLB, had also developed similar ideas. However, as far as I know, Harry's talk was not recorded, so we do not know if he had been able to gain as much insight as WLB. Harry later said that he was confused by crystal structures and that WLB had gone further. WHB was initially more interested in studying the characteristics of X-rays rather than pursuing crystallography, but after a difficult discussion with Rutherford, he reluctantly agreed to leave this field to Moseley and, instead, to concentrate on crystallographic research. WHB then magnanimously offered to help Moseley by explaining the tricks he had developed from his experience in using the spectrometer. At the time, it was not known for sure what the wavelength distribution of X-rays was and that it contained both a broad white component (a continuum of wavelengths) and sharp characteristic lines. In using the spectrometer, it was essential to change the detector angles through very fine steps to avoid missing the sharp lines. Moseley was able to measure the frequencies of the characteristic lines of X-rays for a number of elements, discovering that the square root of the frequency was proportional to the atomic number (the number of protons in the atom). If you ever visit Oxford, you can see his original diagram in the Clarendon Laboratory. This discovery was important because it established the importance of the atomic number and supported the concept of the periodic table, earlier proposed by Dmitri Ivanovich Mendeleev in Russia. It also enabled Harry to fill in some of the gaps in the list of elements in the then known periodic table (see the gaps at atomic numbers 43, 61, and 75.

Moseley's graph for the K and L lines, Clarendon Laboratory Oxford

Moseley had a prestigious talent and was almost certainly destined for a Nobel Prize. However, with the outbreak of the world war in 1914, research ended. Harry decided to show his patriotic duty by enlisting in the army, despite entreaties against this by his family. Calamity struck on the morning of 10 August 1915 during the botched battle of Gallipoli when 30,000 Turks, 'calling upon the name of God', streamed down a hill towards the British lines. According to General Sir Ian Hamilton:

…our men stood to it, and maintained, by many a deed of daring, the old traditions of their race. There was no flinching. They died in their ranks where they stood.

Thus ended the life of a promising young man.

Coincidentally, WHB's son, Robert, was also wounded at Gallipoli on 1 September 1915 and died from his wounds the next day. The effect on WHB and his wife was devastating, something neither of them ever overcame. After the war, in 1920, WHB and WLB were invited to Stockholm for the Nobel Prize ceremony. But WHB refused to go because "there will be Germans there"! His son also did not attend, presumably because of his father's influence, but he did go in 1922.

So, finally, we now come to the poem. Here it is.

BALLAD OF RYERSON

From Edwin H. Lewis (1925). J. Chem. Educ. 2, 610. Copyright 1925 American Chemical Society.

Lo, Paris and Cambridge and Ryerson were needed to make one thought

Till on the final droplet-star, the massiest, tiniest sphere,

The moon-grain lingered a moment and told the secret here.

Now take the charge and the crystal! Young heroes, unlock the lead,

And kindle a rose for mother ere the rose of her hearth be dead.

O planet, ridged with Calvaries and rimmed with Suvla Bays,

Not all your nights are reined with fire, not all of your lightning slays,

Then why have you slain your darlings? And why did your heart dis -

close

Fury and flame and the flash of lead when your dearest brought you a rose?

Ah, the rose! The expectancy and the rose!

The beat of the harp is broken, the heart of the gleeman is fain

To call him back from the grave and rebuild the shattered brain

Of Moseley dead in the trenches, Harry Moseley dead by the sea,

Balder slain by the blindman there in Gallipoli.

No longer the towers of Oxford whisper the middle age,

But the dearest of hopes destroyed and the great unwritten page.

No longer the Trinity meadows bloom as in other days

But the sunlight dreams of violets beyond the violet rays.

Beyond the violet seek him, for there in the dark he dwells,

Holding the crystal lattice to cast the shadow that tells

How the heart of the atom thickens, ready to burst into flower,

Loosing the bands of Orion with heavenly heat and power.

He numbers the charge on the center for each of the elements·

That we named for gods and demons, colors and tastes and scents,

And he hears the hum of the lead that burned through his brain like fire

Change to the hum of an engine, the song of the sun-grain choir,

As it spins the chaliced lightning to banish shadow and shade,

Or drives the heavy hammers by the sun-grain cannonade,

Or wears the wings of the humming birds that flash through heaven afar,

Or grinds the golden barley by the voltage of a star.

Now, if they slay the dreamers and the riches the dreamers gave,

They shall get them back to the benches and be as the galley slaves.

Edwin Herbert Lewis University of Chicago Photographic Archive, apf1-03859, Hanna Holborn Gray Special Collections Research Center, University of Chicago Library.

I see that in his book, White Lightning, published in 1923, Moseley is mentioned thus:

Note Max Laue written on image of the hand

Marvin laid down the magazine and reflected. This unknown Moseley had found it—a sure way to determine the amount of electricity concealed in the heart of any atom. In ten years chemistry would be a new science. In much less than that time every chemical element would receive a number indicating the charge on the nucleus.

Moseley had already numbered some thirty elements, beginning with aluminum as 13, and calculating gold at 79.

So, if anyone out there can fill in more details and throw more light on the reasons for this poem, please let me know.

Oxford

Addendum: Many years ago, I went into the office of one of our secretaries and noticed a cardboard box in the corner behind the door. I also saw that every time someone entered the room, the door was slammed against the box. I looked inside the box, and there was one of Moseley's original X-ray tubes, very similar to the one seen being held by Moseley in the image at the beginning of this article. Miraculously, despite its fragility, it had survived despite its rough treatment. It can now be seen in the small museum of the Clarendon Laboratory.

Remembering Vladimir Koptsik, a theoretician of crystallography and co-author of a famous symmetry book, on his centennial

Istvan Hargittai

Budapest University of Technology and Economics

Vladimir A. Koptsik (1924−2005) was born in Ivanovo, an industrial town, educational and regional administrative center some 250 kilometers northeast of Moscow. He attended school in Moscow and completed the 9th grade in school in June 1941 just as Germany was about to attack the Soviet Union. First, he helped building anti-tank barriers around Moscow, then, for three years, he worked in the defense industry. While working, he completed his school education and enrolled on the correspondent course of the Faculty of Physics of Moscow State University (MSU). In 1944 he became a full-time student of the geophysical department of the Faculty of Geology of MSU. In 1949, he graduated in the Department of Crystallography and Crystal Chemistry and stayed on for PhD-equivalent graduate studies in the same department. Noted crystallographers, such as G. B. Bokii, A. I. Kitaigorodskii, and A. V. Shubnikov were among his professors, and Shubnikov acted as his mentor. Koptsik defended his candidate of science (PhD equivalent) dissertation in 1953. It was at the same time when MSU expanded hugely and took possession of its new campus on Lenin Hills- Koptsik followed Shubnikov to the Faculty of Physics of MSU and helped his mentor organizing the new Department of Crystallography and Crystal Physics.

Vladimir Koptsik lecturing in front of Alexei Shubnikov’s portrait at the Shubnikov Centennial Meeting, 1987, Moscow, and Vladimir Koptsik at the “Symmetry 2000” meeting in Stockholm. Both photographs by Istvan Hargittai

In 1963, Koptsik acquired the higher degree of Doctor of Science, a prerequisite for professorial appointment, which he soon received. 1968, he became head of the department, by now called Department of Crystal Physics. His principal research activities covered theoretical crystal physics, theory and applications of color symmetry, structural phase transitions, and theory of real crystals. He authored and co-authored about 300 publications of original research. He is though best known for his co-authorship of the monograph A. V. Shubnikov and V. A. Koptsik, Symmetry in Science and Art (Plenum Press, New York, 1974) whose Russian original appeared in 1972 [1]. This is also how I met with his name in my symmetry studies and especially while working on our own monograph Symmetry through the Eyes of a Chemist [2]. It was indeed our shared interest in symmetry that initiated our interactions. Koptsik remained active in research of the theoretical aspects of crystallography throughout his career. He published monographs, had 27 pupils having earned the PhD-equivalent candidate of science degree, and creatively contributed to the efforts of the crystallography community both at the domestic and international levels, among others, as a member of the Commission on International Crystallographic Tables of the International Union of Crystallography from 1963−1983. I met Koptsik in person for the first time in 1987 during a conference in Moscow celebrating the one hundredth anniversary of Shubnikov’s birth. His contribution was a panoramic review about generalized symmetry in crystal physics [3]. Our second meeting happened at the “Symmetry 2000” conference where he was one of the invited speakers. Characteristic of his broad interests, Koptsik’s presentation at the Stockholm meeting was about symmetry compositions in the great Russian poet Alexander Pushkin’s works [4].

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PIASA’s Science Awards presented to Eminent Polish-American Scientists at the Kosciuszko Foundation

Author not stated in source

The Kosciuszko Foundation and the Polish Institute of Arts and Sciences of America (PIASA) recently had a joint event honoring distinguished Polish-American scientists Prof. Tomasz Wierzbicki of the Massachusetts Institute of Technology and Prof. Alex Wlodawer of the Center for Cancer Research, National Cancer Institute, Frederick, MD, USA.

The program featured a presentation of the PIASA’s Tadeusz Sendzimir and Casimir Funk Awards to the respective scientists and a short lecture delivered by each laureate. A light reception followed the presentations.

The event was presented as part of the KF Collegium of Eminent Scientists Lecture Series. It was meant for a general audience, free and open to the public..

Prof. Tomasz Wierzbicki: “Aluminum as Main Structural Material on Earth and in Space”

Dr. Tomasz Wierzbicki is a distinguished Professor Emeritus of Mechanical Engineering at the Massachusetts Institute of Technology (MIT). His extensive contributions in the fields of mechanical stability and crashworthiness, spanning automotive, shipbuilding, battery, aluminum, and other industries, have earned him global recognition. Notably, his analyses of the Challenger Space Shuttle breakup, the Exxon Valdez spill, and the World Trade Center aircraft impact and collapse reconstruction have significantly advanced our understanding in these areas.

During his talk at the PIASA Award Ceremony, Dr. Wierzbicki delved into the ubiquitous use of aluminum in our everyday lives, from cars to buildings. He also explored the future of aluminum, particularly its potential as the primary building material for infrastructure on Mars, a topic of increasing relevance in our rapidly evolving world.

Prof. Alexander Wlodawer: “What can structural biology do for human health and the environment.”

Methods employed in the field of structural biology in general, and in the investigation of three-dimensional protein structures in particular, have undergone tremendous changes in the last half-century. Detailed knowledge of such structures is the key to the development of drugs, with the treatment of AIDS providing a textbook example of the successful use of structural information for that purpose. The development of enzymes that can be used to remediate plastic pollution provides another example. Experimental methods used to study protein structures include X-ray and neutron crystallography, NMR (nuclear magnetic resonance), and, more recently, cryo-electron microscopy (cryo-EM). Recent developments of artificial intelligence-based computational approaches to structure prediction, such as AlphaFold, have been truly revolutionary. During his lecture, Prof. Wlodawer illustrated these subjects with examples of work from his laboratory, as well as by other scientists.

Dr. Alexander Wlodawer received his Ph.D. from the University of California, Los Angeles, in 1974. After two years as a postdoctoral fellow at Stanford University, he joined the National Bureau of Standards in 1976 and then moved to the National Cancer Institute in 1978. Until 2020, he was Chief of the Macromolecular Crystallography Laboratory and now is Senior Investigator. Some of the areas of his interest are directly involved in elucidating structural features of molecules that could explain their importance to understanding cancer, AIDS, and COVID-19, but he is also active in the development of methods for protein crystallography. Dr. Wlodawer is a coauthor of 425 publications and serves on the editorial boards of several journals. He was awarded the title of Doctor Honoris Causa by the Technical University of Lodz, Poland, is an elected Foreign Member of the Polish Academy of Sciences, a recipient of the NCI Mentor of Merit Award and of the Heyrovsky Honorary Medal (Czech Academy of Sciences). In 2015, he received the American Association for the Advancement of Science – Foundation for Polish Science Award for Collaborative Research (with Prof. Mariusz Jaskolski).

Robert Langridge (1933-2023)

Suzan Revah

Robert Langridge, PhD, professor emeritus in the Department of Pharmaceutical Chemistry and an icon in the field of molecular computer graphics, passed away just a few weeks after his 90th birthday on November 11, 2023.

Langridge was honored in 2018 with the UCSF Medal, the University's highest honor, for ushering in a new era of biological experimentation and drug discovery. He received the award along with Peter Andrew Kollman, Ph.D., and Irwin "Tack" Kuntz, PhD, in recognition of the group's collaborative spirit and pioneering research in pharmaceutical science and computational chemistry.

In the 1950s, there were two approaches to visualizing molecular interactions: Scientists built wire models, sketched them, and did mathematical calculations. In 1956, Langridge obtained access to an IBM 650 computer. Even though the machine had miniscule memory by today's standards, Langridge loved programming and was able to reduce the computation time of his calculations from two weeks to thirty minutes.

Langridge became convinced that computers were here to stay. "Although there are many stories about Bob's work on the beginnings of molecular computer graphics and how he became this amazing pioneer who recognized the potential of computers, he did that despite the scientific community not being very receptive," said his wife Ruth Langridge, MAT, MA, PhD, a researcher at the University of California, Santa Cruz.

Langridge's 1970 grant for a computer graphics lab at Princeton University established one of the first Research Resource Centers created by the National Institutes of Health. In 1976, he was recruited to UCSF, where he founded and directed the computer graphics lab until he retired in 1994. He pushed the field of pharmaceutical chemistry into the computational era—a daunting task in a time of room-sized computers.

"If you want to see with your own eyes the results of Bob's work, pick out any magazine, video, or movie dealing with science or with many other features of everyday life," said Professor Emeritus of Pharmaceutical Chemistry Kuntz.

Probing biology at the atomic level

Born in the small English village of Froyle in 1933, Robert Langridge was the first in his family to attend university, receiving his BSc in physics at the University of London with first-class honors in 1954. In 1955, he published his first important paper in Nature, detailing the molecular structure of DNA based on x-ray diffraction data.

In 1957, Langridge received his PhD in crystallography from the University of London. His research was guided by Maurice Wilkins, who was studying the structure of DNA using the technique of x-ray diffraction. Wilkins shared the 1962 Nobel Prize with James Watson and Francis Crick for their discovery of the molecular structure of DNA.

As a graduate student, Langridge showed how the Watson and Crick DNA model could be modified to agree with x-ray diffraction studies of DNA. His dissertation on x-ray crystallographic model-building and computational studies of the structure of DNA included the first application of a stored program digital computer (the IBM 650) to the analysis of DNA structure.

Becoming a computational revolutionary

Credit:Christopher Springmann, 1985

After coming to the United States in 1957, Langridge worked as a postdoc in biophysics at Yale University and in biology at the Massachusetts Institute of Technology (MIT). In 1961, he set up a lab to study the structures of DNA and viruses at the Children's Cancer Research Foundation in Boston, with faculty appointments at Harvard University and Harvard Medical School. Concurrently, in 1964 he collaborated on the original work in molecular graphics at Project MAC (now The Laboratory for Computer Science) at MIT.

In 1966, Langridge joined the University of Chicago as a professor of biophysics and then moved to Princeton in 1968 as a professor of chemistry and biochemical sciences. He established the first Computer Graphics Laboratory, the name and concept of which he brought with him to UCSF in the fall of 1976.

"When he came to UCSF from Princeton, he didn't bring any other personnel with him, and he didn't bring any computer hardware with him," said Professor of Pharmaceutical Chemistry Tom Ferrin, PhD, who took over UCSF's Computer Graphics Lab when Langridge retired.

At UCSF, he developed a computer graphics system that produced some of the first pictures of molecular interactions in three dimensions, with the ability to rotate an image on the screen. Among the field's milestones, Ferrin recalled the advent of color graphics as a quantum leap that allowed scientists to identify different chemical components and proteins. "He had to build everything from the ground up, which required a lot of bravery on his part."

"Bob was the son of a gardener who bootstrapped himself up from the ground," added Ferrin, who remembered Langridge as not only a pioneer of molecular computer graphics, but also as an ambassador for the technology. "He had the vision, and he knew that if he was going to realize the vision for his future and make his mark in science, he needed to do that in the United States, which also required a lot of bravery."

The advent of interactivity

The ability to interact with graphic images was the breakthrough that allowed the viewer to gain insight into both molecular structure and function. This resulted from significant effort to develop software that could "meaningfully" display large molecular structures, like DNA and proteins.

"Interactive molecular graphics has always been the key to what we've done at UCSF, which is to make the user part of the graphics system…and allow the user to apply their knowledge and investigate parts of the molecular structure," said Ferrin. "That wouldn't be possible if you're just looking at a drawing or an image on a printed page."

Today's UCSF scientists carry Langridge's legacy forward with computational innovations allowing them to screen millions of potential drugs simultaneously and observe molecular interactions in virtual reality.

"Bob's expertise was in visualization because computations alone just yield columns and columns of numbers. The insight comes from understanding what these computations mean," Ferrin said. "There are countless antecedents along the way, but some brilliant scientists have come to the graphics lab, and they just haven't yet seen the molecules that they're so familiar with in an interactive 3D fashion, and then they'll get some flash of insight from being immersed inside these complex 3D molecules, so it's a very powerful technique."

Inspiration and impact

Langridge's work continues to have an enormous impact on scientific discovery. "He was a giant here at UCSF, and his legacy will be long and fondly remembered," said UCSF Chancellor Sam Hawgood, MBBS.

"Looking back, it seems like Bob was always spreading the word about molecular graphics, and he was the perfect person to do it because he was there from the very beginning," said Ferrin.

Langridge served on the Computer and Biomathematics Research Study Section of the National Institutes of Health (NIH) and the Science and Educational Advisory Committee at Lawrence Berkeley Laboratories. He was a member of the NIH Computer Science & Telecommunications Board of the National Research Council and the NIH Council of the National Center for Research and the council representative on the Advisory Committee to the NIH director.

In 1983, Bob collaborated with Industrial Light & Magic, the motion picture visual effects company founded by George Lucas, and used real-time, interactive graphics of DNA to generate the intro to the "Genesis" segment of Star Trek II. In 1989, he was elected fellow of the American Association for the Advancement of Science and in 1990 to the Institute of Medicine of the National Academy of Sciences. In 2005, he was highlighted by Smithsonian Magazine as an innovator who made a difference.

"Computer graphics has become the paintbrush that colors it all," Kuntz said. "I can't tell you what an honor it was to work with him, day after day, for so long."

Teri Klein, PhD, a faculty member in the Department of Biomedical Data Science at Stanford University, described Bob as an incredible mentor and a wonderful human who "was one of a kind, and I have emulated him throughout my academic career."

"He was my inspiration for our center, in science, in leadership, and in humanity," said Ken A. Dill, PhD, distinguished professor at Laufer Center for Physical & Quantitative Biology at Stony Brook University. "I am forever grateful for his brilliant and inspiring vision."

Langridge is survived by his wife; three daughters, Elizabeth, Catherine, and Suzanne; and five grandchildren.

UCSF School of Pharmacy

Prof Patrick J. McArdle (1945-2024)

Anuradha Pallipurath and Andrea Erxleben

Prof Patrick J. McArdle from the University of Galway passed away unexpectedly but peacefully, at home in Galway, surrounded by his family on the 2nd of January 2024, and was laid to rest in Rahoon cemetery, Galway on the 5th of January 2024.

Pat was a professor of inorganic chemistry with expertise in X-ray crystallography and Nuclear Magnetic Resonance (NMR), who has published over 400 papers on a range of topics, from small-molecule pharmaceuticals, organometallics to carbohydrates. Born and raised in Drogheda, Co. Louth, Pat's first job was at his family hotel, The White Horse. He pursued his B.Sc and PhD (1962 – 1969) from University College Dublin (Tautomerism in Some Binuclear Metal Carbonyl Derivatives) and a D.Sc. (1989) from the National University of Ireland Galway (now University of Galway), where he worked until his passing. Pat was also the last academic staff in Galway who gave chemistry lectures in Irish until he retired (as the Head of the School of Chemistry) from teaching in 2010. He was elected to the Royal Irish Academy on his first application in 1998.

Pat's research work initially concentrated on the organometallic chemistry of iron and later included the synthesis and reaction kinetics of quadruply-bonded metal complexes. He started working in crystallography in the early 1980s when the first four-circle diffractometer in Ireland was set up in Galway. He was one of the five founding PIs of the SFI- and industry-funded Synthesis and Solid State Pharmaceutical Centre (SSPC) in 2007. The setting up of this Research Centre, led by Kieran Hodnett at the University of Limerick, was very important for chemistry in Ireland as it was the first research centre funded by SFI which did research in chemistry. In the SSPC Pat's work concentrated on solid-state analysis of pharmaceutical solids, the use of sublimation for crystal growth and cocrystal synthesis, crystal growth mechanisms and theoretical analysis of solid-state interactions. Together with Pavel Karen (Oslo) and Josef Takats (Alberta), starting in 2009, he worked on an IUPAC project that examined the use of the oxidation state in chemistry. After 10 years of effort the first comprehensive definition of the oxidation state was produced together with an 86-page technical report. He was also a member of the IUCr commission that organised the meeting at Hyderabad, India in 2017.

Pat's passing is a great loss for the crystallography community as well as the University of Galway. Having trained under eminent scientists such as Jack Lewis at University College London and Massachusetts (1969 – 1972), Cambridge during his post-doctoral work, Frank Albert Cotton at Texas A&M (1978), Jack Norton at

Princeton and Columbia USA and Guy Dodson at the University of York, UK (1991) on sabbatical, Pat developed a passion for crystallography and contributed serval computational methods for structural analysis. In 1996, he developed and published the ABSEN program to predict all possible space groups in different orientations from an HKL file. He also developed the ORTEX program to visualise ORTEP diagrams interactively. His interest in computing and crystallography led him to develop the OSCAIL software that integrated several crystallographic tools and is widely used in Ireland to date.

Pat was a very hands-on researcher. Having sourced Ireland's first diffractometer in 1981 along with his colleague Desmond Cunningham, a second-hand Hilger & Watts Y290 4-circle diffractometer from Canada, he had the confidence to take it all apart and put it back together in a functioning form. He believed in innovation but also respected heritage. True to this, he never got rid of older goniometer set-ups when the diffractometers were upgraded and used them to train his students. These are still on display in the crystallography labs in Galway and soon to be added to the National Museum of Ireland's National Scientific Instruments Collection. Pat sought to bring a modern influence on the direction of capital spending on facilities in the new Science building in Galway which opened in 1974. In collaboration with Prof. R.N. Butler, this effort also brought the first 100 MHz NMR spectrometer to Ireland which was followed by a 13C spectrometer and the first high-field NMR spectrometer.

Pat was also an innovator who was not afraid of drilling a hole through a vacuum oven to modify it to control the temperature of his sample for the sublimation process to generate single crystals. He believed in sharing the knowledge he gathered. To that end, his youtube channel has tutorial videos for the tools he has incorporated in OSCAIL to how to set up a cyclone vacuum at home for cleaning, and as an avid cyclist, on how to prevent your cycle chain from falling out.

In his colleague Niall Geraghty's words, "Pat is a renaissance man", who could talk about any topic from molecular orbital theory, history, art, opera, film, theatre and politics. He was a man of outstanding intellect and someone who was interested in everything till the end. His very humble and gentle approach made him a great mentor and a great teacher. Reading through his condolences book reveals how many lives he touched and how many people owe their careers to his training.

His dedication was not just to science but also to his family. Pat is survived by his wife Aideen, children Orla, Eoin, Aideen Óg and their families, as well as his siblings and their respective families.

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