



## Report of the Executive Committee for 2021

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### 1. Meetings

The IUCr sponsored the following meetings that were held during 2021:

6th Conference of the Bangladesh Crystallographic Association, Virtual Meeting, 15–16 January;

CCP4 Crystallographic School in South Africa: Data Collection to Structure Refinement and Beyond, Cape Town, South Africa, 22 February – 4 March (originally scheduled for 2020);

2nd International School on Advanced Porous Materials (MOFschool2021) – Virtual Meeting, 21–25 June;

55 Erice School: Molecular Crystal Engineering – Virtual Meeting, 21–25 June;

European Crystallographic School (ECS6), Virtual Meeting, 4–10 July (originally scheduled for 2020);

To.Sca.Land: Total Scattering for Nanotechnology in Al Andalus, University of Granada, Granada, Spain, 20–24 September; and

10th International Conference of the Hellenic Crystallographic Association, Athens, Greece, 15–17 October (originally scheduled for 2020).

The Executive Committee met virtually in March, throughout June, and in July, August, September and October. The Finance Committee met virtually in March and July, to prepare its advice and recommendations on finances, establishment and staff matters.

The most important items of business dealt with by the Executive Committee at its meetings, and in e-mail ballots, were:

editorial policy, pricing policy and subscription rates, approval of appointments of Editors and Co-editors, journals development, Journals Management Board meeting, Special Issues, Plan S and open access, and other matters concerning the IUCr journals; approval of audited accounts for the previous year;

status of existing membership subscriptions and new membership applications; investment policy;

sponsorship and financial support for meetings, young scientists' support, Visiting Professorship Scheme, gender balance of programmes;

progress with Volumes A, A1, B, C, D, E, F, G, H and I of *International Tables* and development of associated software;

*IUCr Newsletter*;

*World Database of Crystallographers*;

*Online Dictionary of Crystallography*; and

promotional activities.

Other items dealt with in this way were:

consideration of publications, jointly with Oxford University Press, in the IUCr/OUP Book Series;

outreach and education, LAAAMP;

Crystallography in Africa;

review of activities of Commissions, creation of a new Commission on Diffraction Microstructure Imaging;

provision of services to and review of activities of Regional Associates;

review of reports of IUCr Representatives on other bodies;

updates from the Committee on Gender Equity and Diversity;

arrangements for the Prague and Melbourne Congresses; and



Swiss registration and taxation.

Items concerning the Chester office were:  
staffing requirements in the IUCr office in Chester;  
office premises;  
risk analysis; and  
office technology.

## 2. Publications

Volume 77 of *Acta Crystallographica*, Volume 54 of *Journal of Applied Crystallography (JAC)*, Volume 29 of *Journal of Synchrotron Radiation (JSR)*, Volume 8 of *IUCrJ* and Volume 6 of *IUCrData* were published.

## 3. Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Appendix D to the Report of the Twenty-Fourth General Assembly and International Congress of Crystallography [*Acta Cryst.* (2020), **A76**, 217–224].

## 4. Work of the Commissions

### 4.1. Commission on Journals

#### 4.1.1. Overview

The reports that follow below summarize the major developments for each journal during 2021. Each reflects the hard work and dedication of the respective Editorial Boards as well as the Managing Editors in Chester. Here, it is appropriate to make some general comments as well as preview a few highlights discussed further in the individual journal reports below.

The Journals Management Board (JMB) comprises the Main (Section) Editors of each journal, the IUCr Journals Commissioning Editors, and also the Journal Managing Editors and other relevant Chester staff. Due to the continuing effects of the pandemic, the JMB met virtually in early July 2021 (and will do so again in July 2022, although a 1-day in-person JMB is also planned, immediately prior to the 2022 ECM meeting, Versailles, France). In addition, virtual meetings of Main and Managing Editors with the Editor-in-chief, and sometimes others, continue to be encouraged to address individual journal developments. While the international conditions for scientific journal publication, together with ongoing effects of the pandemic, continue to present challenges, the IUCr journals have, on the whole, continued to hold their own in terms of quality research publication and impact factor, although there has been a decrease in the number of submissions to some of the journals, which is a concern. During 2021, and ongoing into 2022, several initiatives have been developed to engender new submissions to the journals and encourage the greater dissemination of open science and data. These were reported to the IUCr General Assembly in August 2021 and a few highlights can be briefly updated as follows:

A new section focused on *Electron Crystallography* has been initiated for *IUCrJ*, with the appointment of a new Main Editor (bringing the total to 7), and several new Co-editors.

A new section focused on *Crystal Growth* has been set up for *Acta Cryst. B* to capture more of the strong papers in this area, some of which have been going to competing non-IUCr journals in recent years. This has involved the strong support of the Main Editors, one of the Commissioning Editors, and appointment of new Co-editors.

A new section on *Raw Data Letters* has been set up for *IUCrData*, intended as a first step in broadening the scope of *IUCrData* to meet some of the open data challenges of the modern publishing environment. Again, this has called for the appointment of a new Main Editor and several new Co-editors.

The transition of *JSR* to open access (OA) was completed in 2021, with all new submissions being treated as open access from October 2021, and the journal becoming OA-only from the start of 2022.

The proportion of open-access papers has continued to increase across the hybrid journals, and it is envisaged that some more of these will transition to become fully open access over the next few years, taking into account the OA performance of *JSR*, as well as the other OA IUCr journals: *IUCrJ*, *IUCrData* and *Acta Cryst. E*. Ultimately, for such ventures to be successful, it will be critical to increase the number of submissions and published papers, without compromising paper quality. Together with continuing commissioning efforts to solicit cutting-edge papers, Topical Reviews, and Special Issues, it will take time to see the fruits of the initiatives highlighted above, but IUCr Journals will continue to explore new developments consistent with the goal of open science and open data.

All of the initiatives above have called for the appointment of new Main Editors and Co-editors, and additionally there has been the traditional turnover of Editorial Boards associated with the IUCr Congress triennial timetable. In this connection, we appreciate the willingness of so many retiring Editors to serve for an additional year due to the one-year postponement of the Prague Congress, and we welcome the large number of new Editors consequently appointed over the past year. The IUCr's continuing commitment to furthering diversity has been, and continues to be, reflected as far as possible in the diversity of new Editorial appointment nominations. This includes diversity in geography, background and gender, subject to meeting the scientific scope, interest and range of expertise needs of a given journal's Editorial Board applicable at the time, as well as the commitment of that nominee to serve in the envisaged role on the Editorial Board.

A. J. Allen, Editor-in-chief, IUCr Journals

#### 4.1.2. Reports by Commissioning Editors

*Biology*. In 2021 Roberto Steiner commissioned the following articles for *Acta Cryst. D* and *Acta Cryst. F*:

*Protein structure prediction by AlphaFold2: are attention and symmetries all you need?* [N. Bouatta, P. Sorger & M. AlQuraishi (2021). *Acta Cryst. D* **77**, 982–991].

*A crystal-processing machine using a deep-ultraviolet laser: application to long-wavelength native SAD experiments* [Y. Kawano, M. Hikita, N. Matsugaki, M. Yamamoto & T. Senda (2022). *Acta Cryst. F* **78**, 88–95].

Roberto also commissioned ten articles for a multi-journal Special Issue on room-temperature crystallography, and is editing most of these Special Issue articles. Four articles have been submitted, six more are expected.

*Chemistry*. In 2021 Elena Boldyreva commissioned several articles related to high-pressure crystallography for *Acta Cryst. D*, *Acta Cryst. B* and *Acta Cryst. C*. Elena is finalizing work on a virtual Special Issue dedicated to chemical aspects of high-pressure crystallography.

Elena's activities in 2021 also included participation in editorial meetings and discussions related to *IUCrData* and a new topic related to crystal growth. Elena has also contributed several papers as an author and is reviewing other papers for *Acta B* and *IUCrJ*.

*Materials, Methods and Instrumentation*. Thomas Proffen was selected as the Commissioning Editor for Materials, Methods and Instrumentation in 2020. Activities in 2021 included participation in editorial meetings and discussions related to *IUCrData*. In collaboration with the IUCr Commission on Powder Diffraction, plans to facilitate the publishing of powder-diffraction papers and improved tools for visualizing powder plots were initiated. Two Special Issues are currently under consideration: one on Machine Learning in Crystallography (*Acta A*, *JAC*) and the other on 3D Printing and Additive Manufacturing (*JAC*).

**R. Steiner**, Commissioning Editor, Biology, **E. Boldyreva**, Commissioning Editor, Chemistry, and **Th. Proffen**, Commissioning Editor, Materials, Methods and Instrumentation

#### 4.1.3. *Acta Crystallographica Section A*

*Acta Cryst. Section A* publishes articles reporting advances in the practice and theory of all areas of structural science. As well as traditional crystallography, this includes nanocrystals, metacrystals, amorphous materials and quasicrystals. It also covers electron crystallography, diffuse scattering, pair distribution function studies, time-resolved XFEL studies, cryo-EM, tomography, small-angle scattering, coherent scattering, diffraction imaging, and the structure of strain and defects in materials. We also welcome contributions on advances in analysis tools that are foundational to crystallography, including descriptions and applications of methods, algorithms and software, and the use of emerging computational approaches such as artificial intelligence and machine learning as applied to structural science.

The journal has two sections: *Advances* and *Foundations*. Articles are selected for the *Advances* section based on their likely impact and broad interest. They benefit from rapid publication and may be highlighted by an accompanying scientific commentary, and tend to be our most read and most

highly cited articles. A list of all the *Advances* papers we have published since the section was launched in 2014 can be found at <https://journals.iucr.org/a/services/advances.html>.

Some of the most popular articles we published during 2021 (based on number of downloads and/or citations) were:

*Layer groups: Brillouin-zone and crystallographic databases on the Bilbao Crystallographic Server* [G. de la Flor, B. Souvignier, G. Madariaga & M. I. Aroyo (2021). *Acta Cryst. A* **77**, 559–571].

*Parameterization of magnetic vector potentials and fields for efficient multislice calculations of elastic electron scattering* [K. Lyon & J. Rusz (2021). *Acta Cryst. A* **77**, 509–518].

*Relativistic spacetime crystals* [V. Gopalan (2021). *Acta Cryst. A* **77**, 242–256] with a commentary: *From crystal colour symmetry to quantum spacetime* [M. Bojowald & A. Saxena (2021). *Acta Cryst. A* **77**, 239–241].

*A cloud platform for atomic pair distribution function analysis: PDFitc* [L. Yang, E. A. Culbertson, N. K. Thomas, H. T. Vuong, E. T. S. Kjaer, K. M. Ø. Jensen, M. G. Tucker & S. J. L. Billinge (2021). *Acta Cryst. A* **77**, 2–6].

Lead Article: *Combining X-rays, neutrons and electrons, and NMR, for precision and accuracy in structure–function studies* [J. R. Helliwell (2021). *Acta Cryst. A* **77**, 173–185].

*The role of an objective function in the mathematical modelling of wide-angle X-ray diffraction curves of semi-crystalline polymers* [M. Rabiej & S. Rabiej (2021). *Acta Cryst. A* **77**, 534–547].

*Coordination sequences of crystals are of quasi-polynomial type* [Y. Nakamura, R. Sakamoto, T. Mase & J. Nakagawa (2021). *Acta Cryst. A* **77**, 138–148].

*Macromolecular phasing using diffraction from multiple crystal forms* [M. Metz, R. D. Arnal, W. Brehm, H. N. Chapman, A. J. Morgan & R. P. Millane (2021). *Acta Cryst. A* **77**, 19–35].

*Multipole electron densities and structural parameters from synchrotron powder X-ray diffraction data obtained with a MYTHEN detector system (OHGI)* [B. Svane, K. Tolborg, K. Kato & B. B. Iversen (2021). *Acta Cryst. A* **77**, 85–95] with a commentary: *Nothing trumps good data* [A. A. Pinkerton (2021). *Acta Cryst. A* **77**, 83–84].

Like many of the other IUCr journals, the number of open-access papers we publish has been increasing. We have found that open-access articles are around 4 times as likely to be viewed, and almost twice as likely to be cited, as articles that are not open access. Other factors that boost readership and citations are featuring the article in a scientific commentary (which we find to be particularly beneficial for the more theoretical or mathematical papers), highlighting it on the cover or the home page of the journal, tweeting about it from the journal's account @ActaCrystA, and featuring it in the *IUCr Newsletter* (<https://www.iucr.org/news/newsletter>).

An Editorial published in January 2021 (*Acta Cryst. A* **77**, 1) outlined some simple steps that authors could take to help maintain the relevancy, vibrancy and broader impact of the journal. These include making sure that the crystallographic context of the work is emphasized early on in the article (e.g. in the title, synopsis, keywords or abstract), thus making it

clear who in the materials or structural communities will use it and what they will use it for. We followed this in February with a very well attended virtual meeting of the Editorial Board, where these ideas were explored further. Throughout 2021 all our Co-editors and the staff in the Editorial Office have been encouraging authors to emphasize the broader context of their work, if necessary by requesting that this is done before an article is sent out for review.

Towards the end of 2021 Laure Bourgeois stepped down from the Editorial Board. We were very sorry to lose Laure and would like to thank them for all their hard work for the journal and wish them the best for the future.

We also lost Uwe Grimm, who passed away suddenly in October. The editorial team and Uwe's colleagues at *Acta A* will greatly miss them. An obituary written by Uwe's close friends Michael Baake, Ronan McGrath and Rudolf A. Römer was published in early 2022 [*Acta Cryst. A* **78**, 63–64].

A. Altomare and S. J. L. Billinge, Editors

#### 4.1.4. *Acta Crystallographica Section B*

In 2021 *Acta Crystallographica Section B* continued to publish six issues per year, the number of articles (pages) published in 2018, 2019, 2020 and 2021 being 75 (744), 136 (1227), 117 (1147) and 112 (1054), respectively. These numbers are highly dependent on the number and size of any Special Issues published in a particular year.

Currently, Poland and Russia are the two largest sources of articles submitted to the journal, together accounting for around one-third of the total. We are therefore concerned that some indirect consequences of the invasion of Ukraine may soon have a significant effect on the number of submissions to the journal. These consequences include problems getting submissions from Russian authors reviewed, various bans on Russian scientists publishing in international journals, and the understandable preoccupations of our Polish colleagues with security and refugees. We will monitor the situation closely over the coming months.

Over the period 2016–2021 the rejection rate has usually been around 30%, with one outlier of 43% in 2018, so the value of 28% for 2021 is not atypical. Recently the average article length has varied between about 9.5 and 10.5 pages, despite several articles of around twice that length. In 2021 the average time between submission and publication fell slightly to 4.5 months. The number of open-access papers jumped to 30, over a quarter of the total published, and more than twice the previous average. Except when we can publish exceptionally high-impact articles, the journal's base impact factor is around 2.0 and we anticipate a broadly similar value for 2021.

In the August 2021 issue, we launched a call for submissions describing aspects of crystal growth that are aligned with the general structural science focus of the journal. The launch was announced *inter alia* by a relevant front cover, an Editorial, changes to the *Notes for authors* and the appointment of two Co-editors (Tatyana Bekker and Karah Knope) to expand the relevant expertise on the Board. Possible future developments include a special collection of recent articles on crystal growth

and a Special Issue with new papers. The aim is to make the journal an obvious home for publications related to relevant studies of crystal growth.

A virtual Special Issue on *Quantum Crystallography* (Guest Editors: Piero Macchi and Jean-Michel Gillet) featured authors who all participated in the first quantum crystallography meeting (QCrOM2020) held online in August 2020, collating articles originally published in the journal between June and December 2021. Anticipated Special Issues include *Structure Correlation and Dynamics in Crystals* dedicated to H.-B. Bürgi (Guest Editors: Simon Grabowsky and Mark Spackman) and a virtual Special Issue on *High Pressure Crystallography* across *Acta B/C/D*, *JAC* and *JSR* (Main Guest Editor: Elena Boldyreva). We are very appreciative of the work of all our Guest Editors for their efforts in bringing about these Special Issues. Invited articles and commentaries are regularly sought from prominent scientists, including Keynote lecturers at IUCr Congresses and Regional Associate Meetings.

The journal has been extensively supported by the Chester staff, notably our Managing Editor Amanda Berry, and we wish to record our appreciation for all their help and advice.

A. J. Blake, M. de Boissieu and A. Nangia, Editors

#### 4.1.5. *Acta Crystallographica Section C*

During the last 12 months *Acta C* has maintained its drive towards becoming a chemically relevant structural chemistry journal with an appeal to both crystallographers and synthetic chemists. The length of the individual papers has been maintained at just over eight pages per article, as it has been for the last couple of years, reflecting the increased chemistry content (synthesis and range of characterization methods) that appears in each paper. Anecdotally, this has been appreciated by the chemistry community, with a particular interest in molecular organic compounds and their intermolecular interactions, as showed by high numbers of downloads for some papers in this area, together with a slight increase in the overall impact factor towards 1.2, an increase over the previous year.

The overall number of submissions (180) and published papers (105) in *Acta C* has reduced further in 2021, which we believe reflects the continued impact of the global pandemic. However, the rejection rate remains steady at around 40%. A recent analysis of withdrawn and rejected articles in *Acta C* indicates that almost a third are resubmitted and published in *Acta C* and *E*, mostly *Acta C*, a further third are published across a wide range of non-IUCr journals, with the remainder are still unpublished a considerable time after rejection.

While no Feature Articles or Special Issues have been published in *Acta C* in 2021, plans are progressing to publish a Special Issue on *Non-covalent interactions based on the sigma hole*, that Jonathan White is organizing with Professor Lee Brammer and two members of their group, from the University of Sheffield, as Guest Editors. The publication date is likely to be late 2022 or early in 2023.



In 2021 four commentaries were published. These have proved particularly popular with the authors of the articles to which they refer and have helped to promote these papers.

The Review Board of referees that was set up in 2016 continues to work well and these crystallographers provide rapid and high-quality reports that help to maintain a reasonable average publication time of under three months. Members of the Review Board agree to review a certain number of papers each year. The Board is being refreshed and expanded to include a wider range of chemists to provide good-quality reviews of the non-crystallographic aspects of the papers that *Acta C* now publishes.

The team of Co-editors continues to do an excellent job checking submitted manuscripts, selecting referees, accepting or rejecting the papers and carrying out detailed editing of the chemistry and crystallography. In 2021 Yoshiki Ohgo (Japan) retired (after 8 years) as a Co-editor and was replaced by Takashi Ohhara (Japan) in early 2022. Eric Reinheimer (USA) also joined the team of Co-editors in 2021.

The Main Editors would like to thank all the Co-editors and Review Board members, past and present, for their support of the journal. Finally, we wish to express our thanks to the Chester Editorial Office staff, who have maintained an outstanding professional standard throughout the recent turbulent times, and without whose hard work and dedication the journal would simply not exist.

L. R. Falvello, P. R. Raithby and J. White, Editors

#### 4.1.6. *Acta Crystallographica Section D*

The *Acta Cryst. D* impact factor has steadily risen to 7.7 for 2021, indicating increasing impact of papers published in the journal. This increase has coincided with maintenance of a strong number of submissions (186) and a larger number of published papers (146) than for over 5 years, nevertheless maintaining a rigorous rejection rate (20%). Among these papers, there is a notable increase to 133 research papers, and consistent numbers of Feature Articles (1, commissioned to provide our audience with relevant context of the revolutionary AlphaFold structure prediction program), Topical Reviews (3), Editorials (2), commentaries (2) and other (5, including obituaries and other short items). We note a dramatic and welcome increase in the number of open-access papers to 93, representing 64% of published papers. There is no obvious cause of this increase from our editorial practice, so we presume it is a result of transformative publishing agreements.

Special Issues continue to play a positive role for the journal, particularly the recurring series of annual CCP4 and CCP-EM symposia, along with the International Symposium on Diffraction Structural Biology. The timeliness of the Special Issue papers is emphasized by publication in regular issues as soon as they are accepted and typeset, rather than waiting until all the papers in preparation are ready. Once all papers for a Special Issue are available they are also collected in a 'virtual Special Issue'.

The main editorial innovation developed during 2021 and introduced in 2022 is the mandatory submission, for review purposes, of data associated with new structures, to ensure that the IUCr journals maintain their position as a global exemplar for the FAIR publication of biological molecular structures. This initiative, led by *Acta Cryst. D*, was progressed through enthusiastic collaboration with the *Acta Cryst. F* and *IUCrJ* Editorial teams, and communication to the community at the IUCr Congress. New submission guidelines, and more detailed descriptions of minimum information required for publication using the major structural methods, were developed and implemented in the submission portal by the Chester Editorial Office.

Publication times have extended to 5.4 months in 2021 – towards the top end of the historical range. Any specific reason for this is unclear, although publication time does appear to correlate with number of pages published, and in 2021 *Acta Cryst. D* published more papers than the preceding years, with a longer average manuscript length. We note that academic teaching workloads have amplified during the current pandemic, and publication times are driven largely by the time required for refereeing and manuscript revision rather than by the technical editing or typesetting, which are both highly efficient thanks to the excellent work by Louise Jones and Simon Glynn in the Chester office, under the supervision of Executive Managing Editor Peter Strickland and Editor-in-chief Andrew Allen. We are very grateful for their hard work, attention to detail and dedication.

C. S. Bond, E. F. Garman and R. J. Read, Editors

#### 4.1.7. *Acta Crystallographica Section E*

In 2021, the number of submissions and publications decreased by approximately 30% and 28%, respectively, compared with 2020. This reduction follows the general trend of the *Acta* journals, albeit to a higher extent. However, the journal continues to attract papers from across the world, and authors from 55 countries have published in *Section E* in 2021.

The top five countries were the USA (19%), Ukraine (10%), Germany (9%), Turkey (7%) and India (6%). In particular, there was a significant increase in the proportion of papers from Ukraine, and a decrease from India. *Acta E* remains the journal with the highest number of downloads (5.7 million of a total of 12.6 million) among the IUCr journals.

The average publication time, which had dropped to 1.1 months in 2020, has slightly increased to 1.3 months. The average number of pages has remained at 5.1 as in 2020, consolidating the trend of submitting papers describing two or more structures, often analysed with complementary techniques (UV-Vis, NMR, DFT *etc.*). The Section Editors identify articles that do not contain sufficient scientific discussion at the pre-screening stage; these are either transferred to *IUCrData* or resubmitted after the authors have improved the content.

The Section Editors have been actively trying to commission papers that will be widely read and highly cited. A series of such papers appeared in 2019 and 2020, and was enriched in

2021 by a paper on twinning [S. R. Parkin, *Acta Cryst.* (2021). E77, 452–465]. Two further educational papers on space groups and crystallographic symmetries were published in the section ‘Modern approaches and tools for teaching crystallography’ [B. M. Foxman, *Acta Cryst.* (2021). E77, 857–863; S.-L. Zheng and M. G. Campbell, *Acta Cryst.* (2021). E77, 864–866].

As part of an effort to attract to *Acta E* manuscripts dealing with structure determinations from powder diffraction data, as well as time-dependent, variable-temperature experiments *etc.* for other IUCr journals, a task group was set up to work on improvements of powder CIFs. Several meetings have taken place between members of the Commission on Powder Diffraction (CPD) (chaired by Dave Billing), IUCr journal staff, Section Editors and Co-editors. Matthew Rowles produced an updated version of *pdCIFplotter* which handles multiple data sets. Mike Hoyland, Peter Strickland and Nicola Ashcroft will work to interface *pdCIFplotter* for people submitting manuscripts to IUCr journals and for referees’ use. Mike and Nicola will also work on fixing common problems with *checkCIF* for powder CIFs. It is hoped that these improvements and others that are in progress will encourage authors to submit manuscripts with powder diffraction data to *Acta E* and to all IUCr journals.

A tribute Special Issue in conjunction with the *Journal of Chemical Crystallography* was dedicated to the memory of Jerry Jasinski, a long-time Co-editor for *Acta E*; starting in September 2021, the issue has by now collected 14 research papers.

Finally, a Special Issue on Modern Approaches and Tools for Teaching Crystallography is forthcoming, edited by Graciela Díaz de Delgado and Sean Parkin. The scope of this issue is to collect papers that can be used as educational materials for young crystallographers and newcomers to crystallography.

We would like to express our thanks to our Co-editors for their dedication and their excellent work. Many of our long-standing Co-editors have retired recently or are due to retire in the course of 2022. We are therefore planning to look for new candidates, keeping in mind gender balance and geographical spread. As always, we are grateful for the constant and excellent support that we receive from the staff in Chester, particularly Gillian Holmes, Sean Conway and Mike Hoyland, for their constant help and support, and Peter Strickland for sound advice and expert guidance.

**G. Diaz de Delgado, C. Massera, S. Parkin and L. Van Meervelt, Editors**

#### 4.1.8. *Acta Crystallographica Section F*

*Acta Crystallographica F* is a home for short and rapid structural biology communications, welcoming manuscripts covering a range of techniques, including crystallography, cryo-electron microscopy, NMR spectroscopy, SAXS and computational approaches. Preliminary results, such as crystallization notes, are only accepted if the system studied is

novel, or if the method has new aspects that may be useful for researchers working on other systems.

In 2021, the journal published 64 papers. This number has continued to fall in recent years and is the result of a decrease in the number of papers submitted. The overall number of pages has also decreased to 483, but the average paper length has increased to 7.8 pages, probably due to the extra scientific requirements for publishing in *Acta Cryst. F*. The average publication time has stayed at a low average of 2.8 months. Accepted papers undergo prompt final editing and usually appear published online in a matter of days, thanks to efficient handling by the Editorial Office in Chester.

No new Co-editors were appointed in 2021 but the current team of Co-editors has good geographical diversity and subject diversity. It would be good to recruit two or three new Co-editors, including one with expertise in cryo-electron microscopy.

The referee panel continues to function well. This group of about thirty experienced scientists have agreed to referee twelve papers a year each, to reply to requests promptly and to return reports within two weeks.

The strengths of the journal include the fast but high-quality scientific and technical editing, its standing in the crystallographic community and its goodwill, by virtue of it being a scientific society journal. However, the impact of the journal and its familiarity to non-crystallographic structural biology communities need to be increased further.

Although the bulk of publications remain Research Communications, nine Methods Communications were published in 2021, an increase from four in 2020. Apart from these, one Editorial, one Commentary and one Topical Review were also published.

The impact factor has been constant over the last four years, but the five-year impact factor and cited half-life have continued their increase. The fraction of open-access papers has stayed at roughly one-third.

It will be important to continue to grow the journal in terms of quantity and quality of papers, but also to maintain the philosophy of short and rapid communications, to distinguish it from *Acta Cryst. D* and *IUCrJ*. One focus should be communicating its wide scope more effectively within the structural biology community. Commissioning more Topical Reviews would help to achieve this goal, together with continued attention to the quality of the Research and Methods Communications.

**J. Newman and M. J. van Raaij, Editors**

#### 4.1.9. *Journal of Applied Crystallography*

Karena Chapman (Stony Brook University) stepped down as a Main Editor for editorial pastures anew in late 2021. Karena had previously served as a Co-editor from 2014 to 2020. We thank Karena for their valuable and tireless support for *JAC* over many years and we wish them all the best in their new editorial role. Flora Meilleur, who has been a Co-editor since 2015, was subsequently promoted to the three-strong group of Main Editors and complements very well the expertise of the

other two Main Editors. Further appointments of new Co-editors are in progress to ensure the multidisciplinary coverage of the journal. In particular, a broad search was conducted for an additional Teaching and Education Editor, which will be described in detail in the annual report for 2022.

The numbers of papers submitted to and published in the journal in 2021 are similar to the numbers over the previous three years. The rejection rate (~33%), impact factor (~3.3), publication time (~5.75 months) and paper length (~10.5 pages) have also remained fairly stable. There was a significant satisfying increase in the fraction of open-access papers in 2021, almost double the average of the previous five years. Research Articles and Computer Programs continue to be the mainstay of article types, while we do need to encourage more Feature and Lead Articles on emerging subjects to attract a wider readership.

We have noted in earlier reports the increased number of citations that articles describing computer programs may garner. The metrics for articles in any category published within the last 18 months are generally and not surprisingly quite low, but a timely description of an established program with a wide user community can be particularly favourable to the journal. The three most highly cited articles from 2021 have been cited 190, 98 and 24 times to mid-May 2022. The six most highly cited articles published since the start of 2020 are in the categories Computer Programs or CIF Applications.

A virtual Special Issue on magnetic neutron scattering is underway [Guest Editors Sabrina Disch (University of Cologne), Sebastian Mühlbauer (Technical University of Munich), Andreas Michels (University of Luxembourg) and Elliot Gilbert (ANSTO)] and is scheduled for publication at the end of 2022. The cross-journal Special Issue on machine learning is advancing slowly.

**J. Hajdu, G. J. McIntyre and F. Meilleur**, Editors

#### 4.1.10. *Journal of Synchrotron Radiation*

The number of published papers rose slightly by six compared with the previous year and the number of published pages exceeded 2000 for only the second time in *JSR*'s history. Submissions were down to 273 from 299, and the rejection rate remained the same at 24%.

Regarding the Editorial Board, we gratefully acknowledge the work of two members who announced their retirements towards the end of 2021: Main Editor Ingolf Lindau and long-standing Co-editor Steve Heald.

One Special Issue was published in 2021 with selected papers from the 11th International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, a recurring series of Special Issues that have been published in *JSR* every two years since 2002. Forming part of the September 2021 issue, the Guest Editors were again Elspeth Garman and Martin Weik; the issue featured seven Special Issue papers totalling 79 pages.

During 2021, plans for a virtual issue on Physics and Chemistry of Actinides Seen by Synchrotron X-rays were formed by *JSR* Main Editor Kristina Kvashnina. The first

papers were submitted in June, and four papers were published in the November 2021 issue, with the remainder to be published in the first issues in 2022, before being brought together as a virtual issue.

The September 2021 issue also saw the publication of an Editorial written by the *JSR* Main Editors and IUCr Journals Editor-in-chief Andrew Allen that provided details about *JSR*'s move to become a fully open access journal from the start of 2022. Starting from 1 October 2021, authors of all newly submitted papers were asked to agree to payment of the open-access article processing charge, providing their article was accepted. It was interesting to note that *JSR* submissions in October, November and December 2021 did not appear to be affected by this.

We thank the readers of *JSR* for their continued interest and support, the authors for publishing in our journal, and the Co-editors for their great services to the journal and to the community.

**Y. Amemiya, K. Kvashnina and D. Bhattacharyya**, Editors

#### 4.1.11. *IUCrJ*

After record years in 2019 and 2020, the number of submissions to *IUCrJ* was down in 2021. However, the journal continued to establish itself within the wider scientific communities that use results obtained from diffraction methods, and impressions from authors, readers, referees and commentators remain positive.

The impact factor announced for *IUCrJ* in 2021 was 4.8. All submissions undergo preliminary screening by a panel consisting of the Main Editors (Dimitri Argyriou, Ted Baker, Richard Catlow, Henry Chapman, Gautam Desiraju, Sriram Subramaniam and Xiaodong Zou) and the Editor-in-chief (Andrew Allen), and this has helped to provide a rapid and efficient review process. Articles that do not meet the journal's requirement for broad scientific significance are often transferred, with the agreement of the authors, to another IUCr journal. Such transfers are seamless and do not require any further work by the authors.

The six issues of *IUCrJ* published in 2021 have featured papers from a wide variety of areas including biology, chemistry, crystal engineering, cryo-EM, materials, physics and FELs. The number of articles submitted to the journal was 117; a total of 108 papers were published with an average turnaround time of 16 weeks. Articles have been publicized in *IUCrJ*'s social media feeds and by other methods, with 11 articles highlighted via in-depth commentaries.

A total of 39 papers were published in the *Biology and Medicine* section of the *IUCrJ* in 2019, representing approximately 36% of the total papers published. It is evident that the biological sciences are a major source of high-impact crystallographic publications, and it is important that this momentum should be maintained.

*IUCrJ* published 25 papers in the *Chemistry and Crystal Engineering* section in 2021 out of the total of 190 in this section since the inception of the journal in 2014. The chemistry component in 2021 is just about its running average

across all years. The contribution of this section has stabilized, while one would expect more papers in the MOF/COF area and also papers dealing with crystal structure determination using electron diffraction and charge density studies, apart from the always popular area of pharmaceutical cocrystals and polymorphs including the events leading up to their crystallization.

Submissions to the *cryo-EM* section of *IUCrJ* were lower than in 2020, with 7 articles published in 2021. *cryo-EM* publications feature strongly in the list of most read articles in *IUCrJ*, and continue to be well cited.

The other sections of the journal, covering *Materials and Computation*, *Neutron and Synchrotron Science and Technology*, and *Physics and Free Electron Laser Science and Technology* have published 18, 10 and 8 papers, respectively, in 2021.

In 2021, we were sad to report the death of John Spence, Richard Snell Professor of Physics at Arizona State University (Tempe, AZ, USA), Director of Science at the National Science Foundation BioXFEL Science and Technology Center (Buffalo, NY, USA) and Main Editor of *IUCrJ*. John was replaced as Main Editor by Henry Chapman of the Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY. Xiaodong Zou of the Department of Materials and Environmental Chemistry, Stockholm University, was also appointed as a new Main Editor in 2021. Xiaodong Zou will lead a new section on *Electron Crystallography*, which will act as a home within the IUCr journals for high-quality, high-impact papers in this field.

The objective of *IUCrJ* remains to attract high-quality science papers of broad scientific significance from across all the scientific communities that use results obtained from diffraction methods. We hope that you will consider publishing in *IUCrJ* and, by doing so, help to further establish the journal as one of the mainstream comprehensive science journals.

**D. Argyriou, E. N. Baker, C. R. A. Catlow, H. Chapman, G. R. Desiraju, S. Subramaniam and X. Zou**, Editors

#### 4.1.12. *IUCrData*

The number of papers submitted to *IUCrData* dropped by some 30% over the past year from 155 to 108 and the number of published papers fell from 139 to 94 over the same period. Whether this decline correlates with difficulties associated with the global COVID-19 pandemic, difficulties in paying the open-access fee (USD 300), competition from the deposition service with the Cambridge Structural Database or other reasons is not clear.

Submissions to *IUCrData* are handled by four Main Editors (Bill Harrison, Edward Tiekink, Luc Van Meervelt, Matthias Weil) and 12 Co-editors. The average page length of a Data Article in 2021 was 2.8 pages and the publication time averaged 0.9 months; the highest proportion of Data Articles came from the USA (23%) followed by China (14%) and Germany (14%).

The continued decline in submissions noted above is of serious concern and plans to make *IUCrData* a more general

'data journal' were explored in 2021. The introduction of a new section, *Raw Data Letters*, was approved and Loes Kroon-Batenburg was appointed as a Main Editor. *Raw Data Letters* will publish short descriptions of crystallographic raw data sets in the biological, chemical or materials science fields. Development work included identifying core metadata for these articles and developing tools to extract the core metadata and write them in imgCIF format as well as working on example articles.

As always, we are extremely grateful for the outstanding support that we receive from the staff in Chester, above all Gillian Holmes, and to Peter Strickland for their advice and guidance.

**W. T. A. Harrison, L. M. J. Kroon-Batenburg, E. R. T. Tiekink, L. Van Meervelt and M. Weil**, Editors

#### 4.2. Commission on *International Tables*

*International Tables for Crystallography* is a book series published by the IUCr in conjunction with Wiley. Nine volumes designated A (and A1) through H are currently in print. A substantial part of a tenth (I, on X-ray absorption spectroscopy and related techniques) is now available online. The *Brief Teaching Edition* has also been a part of the series; in 2021 it was replaced by a revision so extensive that it has a new name (*Teaching Edition: Crystallographic Symmetry*). The *Symmetry Database* is a related online resource.

While *International Tables* has long been a collection of printed books it is being transformed into an electronic resource. Parts of it became available online starting in 2006. The transition is expected to continue because it allows more material to be included, makes it easier to correct or add material, and is advantageous financially. Printed copies of some volumes (*e.g.*, Vols. A and E) are, however, expected to remain available because so many users prefer a version that they can page through and annotate. So far there has been no online version of the *Teaching Edition* but that possibility is being considered.

The new style for chapters, new templates and a new workflow developed in 2020 have allowed numerous early-view versions of chapters to be published before the volume (so far C and I) is complete. Online access to early-view material is especially appreciated by authors who complete their chapters promptly, and it helps the IUCr meet Wiley's annual target of 10% new or revised content.

The 2020–22 pandemic presented important challenges. The budgets of many institutional libraries have tightened. There is increased pressure for citations of an author's publications, which the series cannot, at least yet, provide. The pressure on scientists to produce more 'countables' has made it difficult to obtain reviews for long chapters. The suspension of in-person crystallographic meetings has hindered the search for new Editors. On the other hand the widespread take-up of video conferencing has allowed much greater contact between Editors and the Chester Editorial Office.

The Chester Editorial Office has been working hard to formulate how *International Tables* might evolve to meet the



current challenges. Discussions with stakeholders took place in 2021 and continue.

Descriptions of activities during 2021 for the individual volumes follow.

*Volume A, Space-group symmetry* (the most recent online edition is dated 2016; Editor Mois Aroyo). New versions of the reflection-condition tables that include the so-called ‘diffraction symbols’ (previously known as ‘extinction symbols’) and the accompanying text of Section 1.6.4 were finally approved and will be added to the online version of Vol. A.

A number of corrections, modifications and improvements of the texts of Vol. A were formulated as a by-product of editing the *Teaching Edition*. Implementation in the online version of Vol. A is planned.

A possible modification of Section 3.1 on crystal lattices is being considered.

*Teaching Edition: Crystallographic symmetry (TE)* (the current edition is dated 2021; Editor Mois Aroyo). The greatly revised *Teaching Edition* (so different that it has a new name and abbreviation) was published in May 2021. An article announcing it appeared in the second issue of the 2021 *IUCr Newsletter*. A very favourable review by Massimo Nespolo appeared in *Acta Cryst.* (A77, 506–508) and also in the third issue of the 2021 *IUCr Newsletter*.

Twenty-eight sample pages of the TE have been made freely available via the *International Tables* website (<https://it.iucr.org/Tc/>). An online version of the whole book will soon be available for a token subscription fee.

*Symmetry Database* server of the Online Edition of *International Tables* (updated continuously; Editor Mois Aroyo). The *Teaching Edition of the Symmetry Database* (TESD) was created following the concepts and ideas developed and agreed upon during 2020. The TESP will provide free access to subscribers to the online version of the *Teaching Edition* book to all current programs of the *Symmetry Database* while limiting the sets of space and point groups to which the programs can be applied to those featured in the book.

Under consideration are possible changes in a few of the *Symmetry Database* programs, namely: (a) modification of the layout (*i.e.*, the presentation) of data for series of groups, (b) extending the set of monoclinic settings that are available online (in accordance with Table 1.5.4.4 of Vol. A), and (c) terminology issues related to the modification of some of the names specifying the program options. Work on fixing bugs and improving the presentation also continued.

*Volume A1, Symmetry relations between space groups* (the most recent online edition is dated 2011; the Editor was Ulrich Müller, who has retired). Attempts to find a new Editor for Vol. A1 have not yet been successful but no major revision seems to be needed at this time.

*Volume B, Reciprocal space* (the most recent online edition is dated 2010; Editor Gervais Chapuis). Three new articles have been received. Referees’ reports have been received for one of them and it is being revised. Getting reviews for the other two has been a problem. Many of the chapters in Vol. B are timeless and so do not need revision.

*Volume C, Mathematical, physical and chemical tables* (the online edition is dated 2006; Editor Richard Welberry). The first chapters (53 pages) of this greatly revised edition have appeared online, with others already being prepared for the same. A steady stream of articles is expected to appear during 2022.

*Volume D, Physical properties of crystals* (the most recent online edition is dated 2013; the Editor was André Authier, who has retired). Attempts to find a new Editor for Vol. D have not yet been successful, but no revision seems to be needed at this time.

*Volume E, Subperiodic groups* (the most recent online edition is dated 2010; the Editor was Danny Litvin, who has retired). In July 2021 Gotzon Madariaga was appointed as Editor of Vol. E.

Gotzon has been thinking about the ‘scanning tables’ in Vol. E, which list, for each space group, the 2D layer groups that describe slices of the 3D structure. The description of these tables needs to be improved, they need to be made easier to use, and some additional material needs to be added. Software has been developed such that the tables could be included in the *Symmetry Database* or some other web application, where they could be more easily searched. If the tables existed in the *Symmetry Database* should they also remain in Vol. E? Should whatever solution is chosen for the layer groups also be applied to the 1D rod groups, for which software has also been written? These questions need careful consideration.

Addition of complete information about the subgroups of the subperiodic groups is also being considered.

*Volume F, Crystallography of biological macromolecules* (the most recent online edition is dated 2012; Editors Liang Tong, Eddy Arnold, and the late Michael Rossmann). The pause in revising Vol. F requested by the IUCr’s Executive Committee has been lifted; planning for the third edition has resumed. The Editors and the Chester Editorial Office have been discussing how to make it possible for the readers to directly cite the volume chapters in their publications. The Editors view that change as very important to their being able to recruit first-rate authors.

*Volume G, Definition and exchange of crystallographic data* (the online edition is dated 2006; Editors Brian McMahon and James Hester). Most of the material describing the updated CIF syntax, dictionary and dREL standards is now complete, and work will shortly begin on updating the material describing applications and practice. The possibility of starting to post early-view chapters is under active discussion with the Chester Editorial Office.

*Volume H, Powder diffraction* (new volume in 2019; Editors Henk Schenk, who has retired, Chris Gilmore and Jim Kaduk). A very thorough and complimentary review of Vol. H by Leopoldo Suescun appeared in the 2021 volume of *JAC* (54, 710–713) and also in the first issue of the 2021 *IUCr Newsletter*. There are plans for a revision, which will include articles that fill ‘holes’ in the first edition and revisions in response to feedback. An Editor to replace Henk Schenk has been identified.

*Volume I, X-ray absorption spectroscopy and related techniques* (new volume; Editors Chris Chantler, Federico Boscherini and Bruce Bunker). During 2021 31 more chapters of the new Vol. I were published online in early-view style, making a total of 45 (~300 pages). The Editors are working to finalize the contributed material so that they can write the introduction and summary.

Further information about the volumes can be found at <https://it.iucr.org> and at the home page of the Commission, <https://www.iucr.org/resources/commissions/international-tables>. The 'Guided Tour' available at <https://it.iucr.org/services/guidedtour/> is highly recommended because it shows what is available electronically. Access to the Tables of Contents of all the volumes is free, as are sample pages (including author lists and prefaces); see the home pages for the individual volumes (e.g., <https://it.iucr.org/A/>).

As always it is a pleasure to thank the staff in Chester, especially Nicola Ashcroft and Simon Glynn, who make such attractive online chapter pages in not one but two formats (html and pdf). Simon has been responsible for the early-view chapters of Vol. I, which have a somewhat different style than in previous volumes. Nicola also turns files into web pages and has the additional responsibility of interacting with the volume Editors, which is done with great tact and wisdom. Several important questions arose in 2021 (e.g., whether to add online access to the TE and if so how to charge for it; how to make authors' contributions more visible and citable) that make use of all the Editorial staff's talents and experience; it is difficult to thank them enough.

Carolyn P. Brock, Chair

#### 4.3. Commission on Aperiodic Crystals

After a year of almost no events, 2021 heralds a return to a more normal state for our Commission. Although the 25th IUCr Congress in Prague was held in hybrid mode, which does not necessarily favour contacts and meetings, the community was again able to share its experiences and results. The two microsymbiosia proposed by our Commission, 'Composite and incommensurate modulated crystals: structural and physical properties' and 'Structure, modelling and properties of quasicrystals', covering a broad landscape of our activities (from stability, structure or relationship with properties), were successful. One fascinating Keynote Lecture directly related to aperiodic crystals and entitled 'State of the art understanding of diffraction from aperiodic crystals' was given by Professor Uwe Grimm.

A special session in the memory of An-Pang Tsai, who passed away on 25 May 2019, was also held during the Congress. It provided an opportunity to trace Professor Tsai's career and essential contributions to the 'quasicrystals' field through presentations by Professor Tsai's colleagues.

The new membership of the Commission (the CAC) for the present triennium was approved by the General Assembly.

Concerning education, the CAC supported a Workshop on Structural Analysis of Aperiodic Crystals as a satellite of the 25th IUCr Congress. It took place from 12 to 13 August 2021

at the Institute of Physics in Prague. This two-day workshop was organized by Vaclav Petricek, Morgane Poupon and Margarida Henriques; it was intended to provide basic knowledge and tools to understand and solve complicated structures (magnetic and modulated crystal structures, and quasicrystals).

A kick-off meeting to launch the International Research Network (IRN) 'Open space between aperiodic order and physics & chemistry of materials' took place in hybrid mode from 3 to 7 October 2021 at Carry le Rouet, France. The objective of this IRN is to foster collaborations between the aperiodic crystal community and those who work on chemical and physical properties of materials. The creation of this network is the logical consequence of the previous meetings held in Nagoya (2015), Annecy (2017) and Sendai (2019), bringing together aperiodic and correlated electron communities.

It should be noted, however, that in the context of the global pandemic, the Commission has decided to postpone by one year the Congress on Aperiodic Crystals, which was to take place in June 2021, to June 2022 in Sapporo, Japan.

Finally, the year 2021 ended tragically for our community with the death of our colleague Uwe Grimm, Professor of Mathematics at the Open University, Milton Keynes, UK, at the end of October. Uwe was a leading mathematical physicist, well known for their work on quasicrystals. They were very involved in the life of our Commission and President of the CAC from 2014 to 2016. The community will undoubtedly miss them.

Olivier Pérez, Chair

#### 4.4. Commission on Biological Macromolecules

The Commission (the CBM) aims to support structural biology and macromolecular crystallography worldwide through scientific exchange, training, and promoting policies that encourage the generation and dissemination of knowledge and technologies.

The CBM representatives to IUCr Congress Program Committee (Diana Tomchick, Andrea Dessen, and Atsushi Nakagawa) worked very hard to assemble the best possible program for the upcoming IUCr Congress in Australia. Their proposals secured one Plenary Lecture and almost all the requested Keynote Lectures and sessions.

There is an ongoing effort to improve the impact factors (IFs) of the IUCr journals. The IF of *IUCrJ* is now ~5.4. The IF of *Nucleic Acids Research* is ~11.5. Scientists have equally easy access to *Acta Cryst. D*, *IUCrJ*, *Nucleic Acids Research*, *Nature* or *Science*. As discussed in the past, two issues are critical: the time between paper submission and publication and the careful selection of keywords. Keywords should be carefully reviewed not only by reviewers but also by the Editor of the paper. The Chair of the CBM is happy to report that the time has been greatly improved. However, it seems that the keywords are sometimes misleading, especially for scientists who are not structural biologists. The CBM Chair personally contacted the authors of several potentially highly cited

**Table 1**  
Survey of target words in PDB deposits and primary citations.

Target word	No. of deposits in PDB with target word in title	No. of primary citations with target word in title	No. of primary citations with target word in title, for which at least one deposit also contains the target word
SARS-CoV-2	2011	628	549
COVID-19	56	40	14
HIV	2793	1352	1124
AIDS	2	9	2
Cancer	201	687	93

manuscripts to convince them to submit their manuscripts to IUCr journals. Authors should be encouraged to use more modern and attractive ways of presenting their work, such as presenting structural results using rich internet applications [Porebski *et al.*, (2020). *Protein Sci.* **29**, 120–127]. The ambitious goal is to double *IUCrJ*'s IF in the next five years and increase the IF of our other biological journals, *Acta Cryst. D* and *Acta Cryst. F*. Authors should inform the press-release office of their respective institutions about papers that may be attractive to the general public. This can also be done by the IUCr.

Another issue is related to frequent discrepancies between the title of the paper and the title of the Protein Data Bank (PDB) deposit, which is misleading for many biomedical researchers attempting to search the PDB. Examination of four target words in the title of the deposit and in the primary citations shows the level of discrepancies between the titles of deposits and the titles of the primary citation (the paper) in the PDB (see Table 1).

Other issues discussed with the PDB include group depositions to the PDB that need adequate presentation and a different archiving protocol [Jaskolski *et al.* (2022). *Protein Sci.* **31**, 784–786; doi: 10.1002/pro.4271].

The Commission members and other interested crystallographers have continued to discuss standards for PDB and data depositions that would help *consumers of the PDB who are not structural biologists* receive information that is easier to understand. The COVID-19 pandemic sped up the development of quality standards due to several groups carefully watching the quality of COVID-19-related structures [Croll *et al.* (2021). *Biophys. J.* **120**, 1085–1096]. Classification of common problems in macromolecular structures is listed in Grabowski *et al.* [*IUCrJ* (2021), **8**, 395–407]. The classification may depend on who is looking at the structure, *i.e.*, a crystallographer or a biologist. For example, non-standardized cell placement should be avoided because it makes it more challenging for scientists without a crystallographic background to compare two or more similar structures. Also, occupancies of waters and metals should be carefully examined as they can mislead biomedical researchers.

The Commission continues working with the Committee on Data (CommDat) on several issues:

(a) In the past, the CBM and the Committee on Data jointly submitted a memorandum to the IUCr Executive Committee and proposed a mechanism for making the results of diffrac-

tion experiments publicly available. This action aimed to achieve better reproducibility of scientific discoveries and ensure that the structures and subsequent publications are of the highest possible quality. Despite several articles that were jointly authored by the Editors of several crystallographic journals and the Chairs of the Committee on Data and the Commission on Biological Macromolecules [*e.g.* Helliwell *et al.* (2019). *IUCrJ*, **6**, 341–343], many researchers treat the deposition of diffraction data (as well as the deposition of the structural model) as a nuisance that can be skipped if not requested by the journal. We should encourage IUCr journals to firmly request that every methodological paper has to provide a digital object identifier (DOI) for deposited original raw diffraction data when they submit an article describing a new structure or a new method. An extensive discussion of the issues is available in the following publications: Grabowski *et al.* (2016). *Acta Cryst.* **D72**(11), 1181–1193; Kroon-Batenburg *et al.* (2017). *IUCrJ*, **4**(1), 87–99; Meyer *et al.* (2016). *Nat. Commun.* **7**, 10882; Baker (2017). *IUCrJ*, **4**, 1–2; and Grabowski *et al.* (2019). *Struct. Dyn.* **6**, 06430. CommDat and CBM jointly supported a Keynote Lecture on this for the IUCr Congress in Melbourne.

(b) Following the suggestion from CommDat and the CBM, the Protein Data Bank implemented a policy of inclusion in the metadata of a deposit the senior author's e-mail address and their work institution. The new policy solved the growing issue of deposits with the phrase 'To be published' as their primary citation. The PDB also provides the ORCID identifier of every deposit author, but not all deposit authors provide this information. Currently, only 14% of deposit authors provide their ORCID identifier when depositing structural models with the PDB.

(c) The Commission Chair continued discussing with some CommDat members on better ways to filter PDB deposits that describe non-standard experiments and how metadata are needed to fully describe some types of experiments. Discussions about high-pressure macromolecular crystallography (HPMX) metadata were initiated between Wladek Minor (CBM), John Helliwell (CommDat), Kamil Dziubek (Commission on High Pressure Secretary), and specialists in the field. In May 2021, at the online kickoff meeting, a working group consisting of Kamil Dziubek, Nathalie Colloc'h (Université de Caen Normandie, France), and Julia Lieske (Center for Free-Electron Laser Science, DESY, Germany) was formed and mandated to work on the topic of standar-

dizing high-pressure descriptors in the macromolecular CIF dictionary and relevant annotations in the PDB. The group is currently working on a proposal to be submitted to the wwPDB, aimed at creating common standards of pressure-related metadata in X-ray crystallography and NMR deposits. The parameters under consideration are the pressure value, calibration method, and description of the experimental techniques (including the type of pressure vessel).

#### *Meetings, workshops, and other outreach activities*

The CBM has recommended support from the IUCr for a number of meetings and workshops that could play an important role by providing resources for teaching or major dissemination of results obtained through macromolecular crystallography.

**Wladek Minor**, Chair

#### 4.5. Commission on Crystal Growth and Characterization of Materials

Andrea Zappettini decided to step down from the position of Chair after serving for 9 years, due to their increased responsibilities and commitments at work. The Commission (the CCGCM) owes a tremendous debt of gratitude to them for their services over the years they served as Chair and for their dynamic leadership. Andrea instigated and set up a ballot to nominate a new Chair and the new members for the Commission. The IUCr Executive Committee and, finally, the IUCr General Assembly confirmed the new composition of the Commission. As a result, the Commission membership was refreshed with an intake of some new consultants and the departure of a couple of consultants. The new composition of the Commission is as on the web pages currently. Geetha Balakrishnan (GB), who became a member of the Commission in 2021, was elected as the Chair. The new Chair took over from Andrea Zappettini soon after the Prague Congress. The Commission is now looking into replacing the Brazilian consultant, who has withdrawn, and also refreshing the membership with active and younger members drawn from the community.

At the 25th IUCr Congress in Prague, the Commission was represented in several microsymbiosia as session Chairs and speakers, some of the symposia being held in conjunction with other Commissions. The Commission members also figured amongst the speakers at the conference. The list below shows the microsymbiosia for the Prague Congress in which the Commission participated:

MS6 Application of electron crystallography to functional materials;

MS45 Frustrated magnetic order and emerging science;

MS62 The mineral/life interface – prebiotic chemistry, biomineralization, advanced biomimetic materials; and

MS98 2D type crystals and their heterostructures.

Juan Manuel Garcia Ruiz was selected as a Keynote speaker: *'The crystal and the rose: On the impact of crystals and crystallography in art and mind'*.

The Commission has been active in its support for schools on crystal growth and characterization, as well as large conferences. They are:

Third European School on Crystal Growth (ESCG3), 20–23 July 2022;

Seventh European Conference on Crystal Growth (ECCG7) to be organized in Paris, France, 25–27 July 2022.

The above meetings were postponed from the previous year due to the pandemic. Currently, several members and consultants of the CCGCM (including the current Chair) are involved in the organization of the School and the Conference with different roles (members of the International Program Committee, the International Scientific Committee, speakers and session Chairs). This level of participation ensures that the core interests of IUCr are well taken care of.

The immediate focus now has turned to the preparations for the forthcoming IUCr Congress in Melbourne in August 2023. GB was chosen as the Commission's representative on the International Programme Committee (IPC) for the Melbourne Congress, which is to meet on 21–22 April 2022.

GB held a virtual meeting of the Commission, inviting all the members and consultants to participate, on the 16 November. This offered all the members the opportunity to meet, to make up for the fact that in-person meetings were not possible for many over 2020 and most of 2021 due to the pandemic.

The Commission members and consultants will now meet to discuss the way ahead – the main event to look forward to is the ICCGE in Naples in 2023, where again our members feature on the main organizing committee and in the other international committees. In the current year, the aim of the Commission members is to look for ideas for schools and workshops around the world to promote crystal growth, especially among early-career researchers.

**Geetha Balakrishnan**, Chair

#### 4.6. Commission on Crystallographic Computing

In 2021 we welcomed Paul Boyle (Canada) as a new member of the Commission. Patrick Mercier stepped down from the Commission at the end of their regular term and we thank them for their work. There were no other changes to the Commission.

At the IUCr Congress in Prague the Commission invited one of the Keynote Lectures and (co-)organized two microsymbiosia. In parallel to the main Congress program, the Commission organized a Crystallographic Software Fayre (organizers Martin Lutz and Claudia Millan Nebot). The Fayre was held in hybrid form (physical and virtual). Authors of crystallographic programs presented the newest developments in 21 tutorials.

As a satellite to the main Congress, the Commission organized a Crystallographic Computing School (1–3 September 2021). The organizers of the school were Claudia Millan Nebot, Jan Rohlicek and Martin Lutz, with support from the



main Congress (Radomir Kuzel). While originally planned to be held physically in Nove Hradý, the School was smoothly converted into a fully online event. It was even possible to have social programs in the evenings. The scientific topic was ‘Eigenvectors and Eigenvalues’, which have many applications in the different fields of crystallography. More than 70 participants and speakers contributed to the School. Modern cloud-based tools were used for the presentations and the collaboration on programming projects.

**Martin Lutz**, Chair

#### 4.7. Commission on Crystallographic Nomenclature

The members of this Commission (the CCN) are the Editors of the Union’s journals, the Editors of the volumes of *International Tables*, the Chair of the IUCr/OUP Book Series Committee, the Chair of the Teaching Commission, the Chair of the Committee for the Maintenance of the Crystallographic Information File Standard, and both the IUCr President and General Secretary. In 2021 the number of members was 54. There were also two appointed consultants.

*Nomenclature problems.* The Commission’s web page invites crystallographers to bring nomenclature problems to the attention of any Commission member. No new matters were brought forward in 2021.

A request dating back to the 2014 Montreal Congress was finally resolved. During that meeting several attendees involved in teaching crystallography asked if the definition of a crystal in the *Online Dictionary of Crystallography* (‘A solid is a crystal if it has *essentially* a sharp diffraction pattern.’) might be expanded to include language easier for beginning students. After considerable debate the definition was expanded to include a direct-space description (‘A solid is a crystal if its atoms, ions and/or molecules form, on average, a long-range *ordered* arrangement.’). The 39 members of the CCN who voted (72% of those eligible) all endorsed the proposal but it was generally agreed that the proposal is an interim solution and should be considered further.

An article about the change appeared in the second issue of the 2021 *IUCr Newsletter*. The article includes some historical material and describes the issues raised by CCN members during discussion of the change.

*Online Dictionary of Crystallography* (the *ODC*). The CCN is responsible for maintaining the *ODC* (the Editor is Gervais Chapuis), which was established in 2006 as a wiki and continues to be run as such, *i.e.*, as a website of definitions that qualified members of the crystallographic community can add to or modify. During 2021 a snapshot of the *ODC* was published in paperback form on the occasion of the IUCr Congress, as had also been the case in 2017 and 2014.

The number of new entries added to the *ODC* in 2021 was small, as was the number of authors who created new entries or revised existing definitions. All attempts to increase *ODC* activity have been unsuccessful.

**Carolyn P. Brock**, Chair

#### 4.8. Commission on Crystallographic Teaching

The Commission (the CCT) continues to be a large, vibrant group with members and member consultants. Since the February 2021 update, the CCT has reviewed additional requests for funding. Despite COVID-19, the turnaround time for evaluation letters has been streamlined to 3 weeks or less. Members of the CCT actively participated in the IUCr Congress in Prague and the new membership roster was confirmed. Planning is underway on educational and crystallography teaching activities in the age of COVID-19 and for the 2023 Congress.

**Oluwatoyin (Toyin) A. Asojo**, Chair

#### 4.9. Commission on Crystallography in Art and Cultural Heritage

The Commission (CrysAC) continues to pursue its mission of spreading crystallographic knowledge related to artworks and ancient materials. 2021 was a recovery year from the 2020 COVID-19 pandemic, though restrictions on travelling persisted and many meetings were cancelled or postponed. The IUCr Congress in Prague marked the partial restart of activities.

The Commission members are G. Artioli (Chair, Italy), S. Bette (Germany), J.M. Delgado (Venezuela), K. Janssens (Belgium), T. Kamiyama (Japan), P.C. Ravines (USA), S. Svarcova (Czech Republic) and E. Tereschenko (Russia), and the consultants are C. Abad-Zapatero (USA), P. Bezdička (Czech Republic), J.-M. Castera (France), M. Cotte (France), E. Dooryhée (USA), E. Makovicky (Denmark), S. Mande (India), S. Quartieri (Italy), A. Rafalska-Lasocha (Poland) and M. Schreiner (Austria).

CrysAC played an active role at the IUCr Congress in Prague, which was for the first time in a hybrid form, combining both on-site and remote attendance.

The Chair of the Commission, Gilberto Artioli, provided a Keynote Lecture ‘Crystallography and cultural heritage – On beauty, science, and passion’.

MS-78 ‘Science meets art: X-ray spectrometry and X-ray diffraction in art and archaeology’ was co-chaired by Gilberto Artioli (remotely) and Sebastian Bette (on site).

MS-85 ‘Science meets art: Crystallography and cultural heritage’ was chaired by Petr Bezdička (on site) and opened with an invited lecture by Koen Janssens, who presented the potential of MA-XRD in the fingerprinting of natural ultramarine. In the same session Silvie Švarcová and Sebastian Bette described secondary degradation products affecting the stability and appearance of artworks. All extended abstracts of the presentations are included in the Congress issue of *Acta Crystallographica Section A*, Volume 77.

At the workshop ‘Novel physical and chemical methodologies for the conservation and restoration of cultural heritage’ in October 2021, Accademia Nazionale delle Scienze detta dei XL, Rome, Gilberto Artioli delivered an invited lecture on ‘Unusual mechanisms of blue colouring in art and

archaeological materials: crystal-chemical aspects' (<https://www.youtube.com/watch?v=Mdm3DVyfKkY>).

Silvie Švarcová organized the seminar/webinar 'Metal Soaps in Paintings: History, Chemistry and Crystallography' at the Institute of Inorganic Chemistry of the Czech Academy of Sciences on 13 July 2021, and on the occasion of the visit of Dr Joen Hermans (Rijksmuseum & University of Amsterdam, The Netherlands) to the ALMA laboratory. It was dedicated to the study of degradation processes that seriously damage the appearance and stability of paintings.

At the International Festival of the Nuragic Civilization, V Edition, Orroli, Sardinia, Italy, Gilberto Artioli delivered an invited talk on 'Lead isotope ratios applied to Sardinian tin metal objects', 10–12 September 2021 ([http://geo.geoscienze.unipd.it/cristalli/video/Orroli\\_Round%20Table\\_%20Artioli.mp4](http://geo.geoscienze.unipd.it/cristalli/video/Orroli_Round%20Table_%20Artioli.mp4)).

At session 145-T105 ('Reading the Record of Volcanic Tephra and Tuff in Geoarchaeological Site Studies and Drill Core Records') of GSA Connects 2021, Portland, Oregon, Gilberto Artioli delivered a talk with the title 'Ancient pozzolanicity revisited: novel insights on materials and reactive processes of Roman hydraulic binders' on 12 October 2021 (<https://gsa.confex.com/gsa/2021AM/meetingapp.cgi/Session/51738>).

In February 2021, Gilberto Artioli delivered a seminar on 'Mineralogy, crystallography, art and archaeology: Science and passion' within the framework of the 'UniPadova Incontra' program for high-school students, Liceo Classico Majorana Corner, Mirano.

The Commission is also responsible for updating the CrysAC website at <https://www.iucr.org/resources/commissions/crysac>.

**Gilberto Artioli**, Chair

#### 4.10. Commission on Crystallography of Materials

The Commission website is <https://www.iucr.org/iucr/commissions/crystallography-of-materials>.

Members: Changqing Jin (Chair, People's Republic of China), A. Abakumov (Russia), V.A. Blatov (Russia), Y. Gogotsi (USA), C. Grey (UK), H. Hosono (Japan), S. Pan (People's Republic of China) and M. Petrukhina (USA). Consultants: M. Fantini (Brazil), H. Maynard-Casely (Australia), A.R. Oganov (USA), Y. Sugawara (Japan), I. Troyan (Russia), O. Yaghi (USA), Nan Zhang (People's Republic of China) and X.F. Zhou (People's Republic of China).

##### *Conferences and symposia organized by members*

Hideo Hosono: Chair, The 2nd Materials Research Meeting (Yokohama, 12–16 December). Hybrid. Number of participants: ~1800.

Changqing Jin: Organizing Committee Member, The 8th National Conference on Crystallography of China (21–24 October 2021). Number of participants: ~1800. Symposium Co-chair, The 2021 European Materials Research Society e(EMRS) Conference. Number of participants: ~2000 (<https://www.european-mrs.com/emergent-functional-materials-respect-extreme-conditions-emrs-0>). Symposium Co-chair,

Conference of China Materials Research Society (8–12 July 2021). Number of participants: ~800 (<https://cmc2021.scimeeting.cn/cn/web/index/>).

Artem Oganov: 20th Workshop on Crystal Structure Prediction with USPEX Code, Skolkovo Institute of Science and Technology, Moscow, Russia, 17–19 November 2021. Number of participants: >100, <https://uspexschool2021.skoltech.ru>.

Marina A. Petrukhina: ACS Symposium 'Petroleum Research Fund at 65'. The 262nd National Meeting of the ACS, Atlanta, 22 August 2021 (virtual).

O. Yaghi: Organized the 21st Century Materials Emerging Scholars at the Frontiers Symposium, virtual meeting, 8–10 November 2021.

##### *Disseminating knowledge and technical skills*

A. Abakumov: VI International School/Conference of Young Scientists 'Solid state chemistry of battery materials', Skoltech, Moscow, 12–16 November 2021, organized by Professor A. Abakumov, E. Antipov and K. Stevenson, <https://crei.skoltech.ru/cest/conference-of-young-scientists-2021/>. Number of participants ~50.

Xiang-Feng Zhou: The 2nd Forum of Young Scholars for Metastable Materials, 28–30 May, Qinhuangdao, China. <https://mmlab.yzu.edu.cn/info/1011/1647.htm>.

Y. Gogotsi: MXene certificate course online: <https://nano.materials.drexel.edu/mxene-course/>. Held twice in 2021: 22–26 March and 2–6 August. About 60 registered participants in each.

**Changqing Jin**, Chair

#### 4.11. Commission on Diffraction Microstructure Imaging

August 2021 saw the approval of the Diffraction Microstructure Imaging (DMI) Commission at the 25th IUCr Congress in Prague. The DMI Commission aims to serve a growing, diverse community of researchers traditionally supported by the IUCr including physicists, materials scientists, and imaging scientists in addition to groups typically not associated with the IUCr including mechanical, civil, aerospace, and nuclear engineers. All share a common goal of understanding materials at the mesoscale and how this mesoscale structure ultimately affects the properties of materials in order to better use existing materials systems and guide the creation of next-generation materials. The tools of this community are diffraction-based characterization techniques capable of non-destructively probing spatial variation of structure in 3D, such as differential aperture microscopy, 3D X-ray diffraction, and energy dispersive diffraction. While these techniques have been developed at national neutron and synchrotron facilities, they are poised for transfer to laboratory settings due to advances in source and detector technology, greatly expanding their global reach. The DMI Commission is tasked with developing standards, educational materials, and growing this international community of researchers.

The Commission members and consultants are practicing users of DMI techniques from around the world: Chair,

Darren Pagan (The Pennsylvania State University, USA); Secretary, Ulrich Lienert (Deutsches Elektronen-Synchrotron, Germany); Community Development Officer, Ashley Bucsek (University of Michigan, USA); Leyun Wang (Shanghai Jiao Tong University, China); Reeru Pokharel (Los Alamos National Laboratory, USA); Masakazu Kobayashi (Toyohashi University of Technology, Japan); Erik Lauridsen (Xnovo Technology, Denmark); Sébastien Merkel (Université de Lille, France); and Henning Friis Poulsen (Denmark Technical University, Denmark).

The consultants are: Matthew Miller (Cornell University, USA), Paul Shade (Air Force Research Laboratory, USA), Henry Proudhon (MINES ParisTech, France), Jun-Sang Park (Argonne National Laboratory, USA), Jon Tischler (Argonne National Laboratory, USA), Jon Wright (European Synchrotron Radiation Facility, France), John Daniels (University of New South Wales, Australia) and Justin Kimpton (Australian Synchrotron, Australia).

The full Commission and consultants meet on a monthly basis and formation of sub-committees including physical standards, data standards, and community outreach has begun. A website for the DMI Commission has been created and can be accessed from the IUCr web page. The website provides information about the Commission, educational materials for new researchers, and updates for the community including upcoming workshops and job postings. A growing mailing list has also been created to provide researchers with information about Commission activities. Upcoming focuses for the next year are the further development of sub-committees, creation of a young scientist connection platform, and holding the first DMI workshop. After meeting, the Commission has voted that development of novel reconstruction techniques using limited projections and multicrystal structural determination and refinement are the first target science thrusts for the DMI Commission to support and pursue.

**Darren Pagan**, Chair

#### 4.12. Commission on Electron Crystallography

Members: M. Gemmi (Chair, Italy), K. Balzuweit (Co-chair, Brazil), L. Bourgeois (Australia), T. Gorelik (Germany), D. Jacob (France), K. Komatsu (Japan), P. Moeck (USA), A. Stewart (UK), Jun Liang Sun (People's Republic of China), H. Young (Canada) and M. Zubko (Poland).

Consultants: P. Van Aken (Germany), J. Bruhn (USA), J. Ciston (USA), F.G. Coury (Brazil), D. Van Dyck (Belgium), J. Hadermann (Belgium), S. Haigh (UK), A. Kirkland (UK), S. Kodjikian (France), U. Kolb (Germany), Q. Li (China, People's Republic of), L. Meshi (Israel), B. Nannenga (USA), L. Palatinus (Czech Republic), H. Xu (Sweden) and X.-D. Zou (Sweden).

The major goals of the Commission on Electron Crystallography (the CEC) are the teaching and promotion of electron crystallography science.

During our meetings in 2021 most of the discussions were focused on the organization of the next IUCr Congress in Melbourne. The CEC has chosen Laure Bourgeois as its

representative on the Programme Committee. There have been proposals of possible microsymbiosia and Chairs and invited speakers. The CEC appointed some new members (M. Gemmi, T. Gorelik, K. Komatsu, A. Stewart, J. Sun, M. Zubko) and new consultants were added. A new Chair was also chosen (M. Gemmi).

During the IUCr meeting in Prague there were more than ten electron crystallography symposia, which were well attended. There were three Keynote Lectures related to electron crystallography, given by Lukas Palatinus (consultant), Edgar Rauch and Tamir Gonen.

At the IUCr meeting in Prague the previous Chair of the CEC, L. Meshi, awarded the Gjønnnes medal in electron crystallography to U. Kolb and S. Hovmöller.

##### *Workshops/schools on electron crystallography*

Damien Jacob (CEC member) participated in the organization of the third edition of the CrystElec school, which took place in Grenoble, 11–15 October 2021. This school focused on the determination of structures and microstructures at the nanometric scale by electron diffraction in a transmission electron microscope (TEM), and was supported by the French Society of Microscopies (SF $\mu$ ) and the LABEX CEMAM.

Jessica Bruhn (CEC consultant) was one of the instructors for the 2021 American Crystallographic Association Workshop 5: MicroED of Small and Macromolecules. This workshop was organized by Tamir Gonen (UCLA) and Brandon Mercado (Yale). It was virtual with 50–100 participants. Jessica also prepared a data-processing tutorial for small-molecule 3D ED/MicroED data using DIALS with the help of David Waterman. This is available on the DIALS website: <https://dials.github.io/documentation/tutorials/3DED/Biotin.html>.

Junliang Sun (CEC member) supervised the organization of the electron microscopy session at the CCRS Congress, Nanchang, China.

Tatiana Gorelik (CEC consultant) gave a series of lectures and tutorials on electron crystallography at Novosibirsk State University, Russia, in February and March 2021, and organized a workshop on ePDF as a satellite meeting to the IUCr Congress, held online 1–2 September 2021. Dr Gorelik, as Chair of SIG4 of the ECA, also organized the 6th ECA Lunch Webinar by Hosea Nelson, titled 'Applications of electron diffraction in organic chemistry', held online 9 December 2021.

Karla Balzuweit (CEC consultant) was part of the Scientific Commission for the organization of two microsymbiosia dedicated to electron diffraction at the biannual Congress of the Brazilian Society of Microscopy and Microanalysis, 28o. Congresso da Sociedade Brasileira de Microscopia e Microanálise, held online 12–15 July 2021. Karla also organized a pre-Congress 8-hour introductory-level course CS02 Difração de elétrons: conceitos básicos, detalhes experimentais e aplicações práticas, held 5–8 July 2021.

Maciej Zubko (CEC member) reports that in 2021 two meetings related to electron crystallography were held in Poland: the XXV Seminar of the Polish Society of Materials Science, 24–27 October 2021, Arłamów, Poland, with approximately 100 participants; and the 62nd Polish Crystal-

lographic Seminar, 24–25 June 2021, an online meeting, with approximately 100 participants. Maciej also prepared lectures on electron crystallography for the PhD students of the International Ecological Doctoral School conducted by the University of Silesia in Katowice, 15–17 March, which had approximately 15 participants.

Xiaodong Zou (CEC consultant) participated as a teacher in an Introductory Course to Three-Dimensional Electron Diffraction (Royal Society of Chemistry), 12–15 April 2021, via Zoom. More than 350 people participated in the event, organized by Dr Zhehao Huang, Dr Tom Willhammar, Dr Hongyi Xu and Professor Xiaodong Zou (Stockholm University). Together with Dr Hongyi Xu (Stockholm University), Dr Lukas Palatinus (Institute of Physics, Czech Academy of Science; consultant) and Professor Louisa Meshi (Ben Gurion University of the Negev; consultant), Professor Zou organized the ‘Electron crystallography school’ at the 25th IUCr Congress (hybrid format), 11–14 August 2021 via Zoom and at the Prague Congress Centre, with more than 200 participants from 46 countries. Xiaodong Zou was also Co-chair of the Microcrystal Electron Diffraction session at ACA2021 (virtual meeting), 31 July 2021.

Mauro Gemmi (CEC member) gave a lecture ‘3D Electron diffraction: the nanocrystallography revolution. Applications to pharmaceuticals and macromolecules’ at the school ‘Unravelling the Complexity of Biological Systems by Electron Microscopy’ held online in Como, Italy, 19–20 April 2021.

#### *New developments and perspectives*

The advent of 3D-ED has increased the number of structures solved using electron diffraction data. This requires setting up guidelines for CIF files specific for electron diffraction that avoid the standard alerts that would be relevant for X-ray diffraction. Members M. Gemmi and T. Gorelik, and consultants X. Zou, J. Hadermann and L. Palatinus are part of the NanED ITN European project on electron nanodiffraction together with the IUCr as a partner, and together they will work to adapt the CIF architecture to the new needs of 3D electron diffraction.

#### *Activities related to IUCr publications*

Owing to the increasing importance of electron crystallography, the IUCr decided to devote a dedicated section of *IUCrJ* to this subject. The Main Editor of the *IUCrJ* electron crystallography section will be Xiaodong Zou (consultant), while Mauro Gemmi (member and Chair), Junliang Sun (member) and Louisa Meshi (consultant), together with Peter Nellist and Jose Rodriguez, will be the Co-editors. This is a great achievement for the CEC.

The Commission has a website maintained by A. Stewart (member): <https://www.iucr.org/resources/commissions/electron-crystallography>.

**Mauro Gemmi**, Chair

### 4.13. Commission on High Pressure

In February 2021, the online 2021 IUCr High Pressure Workshop was organized by the local team of Professor Elena

Boldyreva and Dr Boris Zakharov, and based in Novosibirsk, Russia. Despite being held in the middle of the COVID-19 pandemic, the workshop (which was first fully virtual event organized by the Commission) attracted 353 participants from 27 countries and proved to be a great success. A comprehensive report of the workshop can be found at [https://www.iucr.org/news/newsletter/etc/articles?issue=150867&result\\_138339\\_result\\_page=23](https://www.iucr.org/news/newsletter/etc/articles?issue=150867&result_138339_result_page=23).

As an immediate outcome of the workshop, Professor Boldyreva became an Editor of an IUCr Journals Virtual Special Issue on High Pressure Crystallography, which consists of a collection of original Research and Feature Articles.

Haozhe Liu, the CHP Chair and a member since 2008, ended their term and stepped down both as Chair and a member, but remained in the Commission as a consultant. The Commission elected a new Chair, Kamil Filip Dziubek (Italy) and Secretary, Boris Zakharov (Russia). Two CHP members, Jean-Paul Itié and Yasuo Ohishi, stepped down from the Commission. The CHP also welcomed new members: Amy Jenei (USA, a former CHP consultant), Kazuki Komatsu (Japan) and Wenge Yang (People’s Republic of China). There are also new consultants: Agnès Dewaele (France), Giovanni Hearne (South Africa), Yongjae Lee (South Korea) and Timothy Strobel (USA). The IUCr General Assembly approved all the changes at the meeting held during the IUCr Congress in Prague. The updated list of CHP members and consultants is available at: <https://www.iucr.org/resources/commissions/high-pressure/members>.

The CHP had participated in the Prague IUCr Congress Programme Committee and had supported two Keynote Lectures (given by Leonid Dubrovinsky ‘High-pressure crystallography unlimited’ and by Yanming Ma ‘Record high superconductivity in sodalite-like rare-earth hydrides stabilized at high pressures’). There were also two microsymbiosia proposed by the CHP: MS-83 ‘High pressure crystallography’ (Chairs: Lars Ehm, Jon Eggert, Vitali Prakapenka and Przemysław Dera) and MS-102 ‘Crystallography using large volume presses and diamond anvil cells’ (Chairs: Shanti Deemyad and Ronald Miletich). Two other microsymbiosia proposed by other Commissions were supported by the CHP: MS-70 ‘Matter at extreme conditions at SR and XFEL: complementarity of spectroscopy and diffraction’ (proposed by the Commission on Synchrotron and XFEL Radiation; Chairs: Angelika Dorothea Rosa and Ulf Zastrau) and MS-61 ‘Magnetic structures at extreme conditions and in extreme samples’ (proposed by the Commission on Magnetic Structures; Chairs: Angel M. Arevalo-Lopez and Andrzej Katrusiak).

After the IUCr Congress in Prague, the incoming CHP Chair organized an online business meeting. The most salient issues included the venue of the 2022 IUCr High Pressure Workshop, identifying the representation to the International Program Committee (IPC) of the 2023 IUCr Congress in Melbourne and progress on the high pressure data management requirements and metadata standards. Kamil F. Dziubek was nominated to act as the representative to the IPC. A full report of the online CHP meeting can be found at <https://>



[www.iucr.org/resources/commissions/high-pressure/minutes/2021\\_minutes](http://www.iucr.org/resources/commissions/high-pressure/minutes/2021_minutes).

It was decided by the Commission in a vote by the members to organize the 2022 IUCr High Pressure Workshop in APS at Argonne, USA. Seven out of 10 members voted in favour of this nomination. The APS scientists Dr Vitali Prakapenka and Dr Stella Chariton kindly agreed to act as the core of the local organizing committee. The meeting is going to be held in September 2022 and the task of preparation is ongoing.

A working group dealing with 'standardizing' high pressure data in chemical crystallography was established (Ross J. Angel and Kamil F. Dziubek – IUCr Commission on High Pressure; Simon Coles, John R. Helliwell, Amy Sarjeant – CommDat; James Hester – COMCIFS; David Allan – Diamond Light Source; Mathias Meyer – Rigaku). The working group constantly moves toward the aim of proposing a high pressure CIF dictionary.

**Kamil Filip Dziubek**, Chair, and **Boris Zakharov**, Secretary

#### 4.14. Commission on Inorganic and Mineral Structures

There were a number of changes to the Commission (CIMS) at the 25th IUCr Congress in Prague. Chris Ling (Australia) became Chair, while Jose Luis Jordá (Spain), Anna Gągor (Poland), Emma McCabe (UK), Kazumasa Sugiyama (Japan), and Serena Chiara Tarantino (Italy) were all welcomed as new members. Patrick Mercier (Canada) stepped down as Chair, and Peter Burns (USA), Frédéric Hatert (Belgium), Roberta Oberti (Italy), Marek Wołczyr (Poland), and Akira Yoshiasa (Japan) stepped down as members and were all thanked for their outstanding service.

All current members and consultants are listed below along with their other relevant roles in the IUCr and the scientific community more broadly.

Members for 2021 to 2023: Chris Ling – Chair, Australia (Consultant, Commission on Structural Chemistry; Past President of the Society of Crystallographers in Australia and New Zealand; Member of the National Committee for Crystallography of the Australian Academy of Science); Jose Luis Jordá, Spain; Marie Colmont, France; Anna Gągor, Poland; Volker Kahlenberg, Austria; Emma McCabe, UK (Secretary, Neutron Scattering Group of the Royal Society of Chemistry and the Institute of Physics); Massimo Nespolo, France (Consultant, Commission on Crystallographic Nomenclature; Member, IUCr/Oxford University Press Book Series Selection Committee; Editor-in-chief, SpringerBriefs Series in Crystallography; Associate Editor of the *European Journal of Mineralogy*; Member of the Advisory Board, *Crystal Research and Technology*); Kazumasa Sugiyama, Japan; Serena Chiara Tarantino, Italy; and Natalia Zubkova, Russia. Consultants: Christopher Cahill, USA; Giovanni Ferraris, Italy; John Parise, USA; Isabella Pignatelli, France; Dhananjai Pandey, India (Member, Commission on Journals; Co-editor, *Journal of Applied Crystallography*); Sergey Krivovichev, Russia; K. (Byron) Byrappa, India; João Rocha, Portugal (Consultant, Commission on NMR Crystallography and Related Methods); Patrick Mercier, Canada; Thorsten Gesing, Germany; Mark

Welch, UK; Marius Ramirez Cardona, Mexico; and Roberta Oberti, Italy (President, European Mineralogical Union; Italian Representative, International Mineralogical Association).

Beyond the ongoing roles listed above, CIMS members and consultants were active across their national and related international communities. Of particular relevance is that the International Mineralogical Association (IMA) has proclaimed 2022 the Year of Mineralogy. This is supported by the United Nations but is supported and formally approved by UNESCO. It will be celebrated as part of the UN International Year of Basic Sciences for Sustainable Development, IYBSSD2022. The IUCr is formally supporting these initiatives and Michele Zema, the IUCr Executive Outreach Officer, is a member of the Steering Committee. This is an excellent opportunity for the IUCr to strengthen the collaboration with the mineralogical community, and CIMS members and consultants are taking the lead.

Chris Ling is a member of the International Program Committee for the 26th IUCr Congress (Melbourne, Australia, August 2023).

Giovanni Ferraris is a member of the Organizing Committee for the meeting Quasicrystals: State of the Art and Outlooks at the Italian National Academy of Lincei, Rome, Italy (rescheduled due to COVID-19, now 18 November 2022).

Roberta Oberti and Giovanni Ferraris are organizing the meeting Mineralogical Sciences and Materials for Sustainable Development, which will be held at the Accademia delle Scienze in Turin, 24–25 May 2022; this is one of the official activities in Italy for the International Year of Mineralogy, in the framework of the International Year of Basic Sciences for Sustainable Development (IYBSSD) recently approved by the UN.

Roberta Oberti (consultant) collaborated with the International Mineralogical Association (for which they are the Italian representative) for the organization of the International Year of Mineralogy.

Isabella Pignatelli will be involved in the school Analyse Structurale par Diffraction des Rayons X sur Monocrystal et Applications (Nancy, France, 3–7 July 2022).

Anna Gągor was an organiser of the 62 Konwersatorium Krystalograficzne (62nd Crystallographic Seminar) of the Polish Academy of Sciences and the Polish Society of Crystallography, held online, 24–25 June 2021.

**Chris Ling**, Chair

#### 4.15. Commission on Magnetic Structures

##### *Membership changes*

Because the IUCr Congress and General Assembly (GA) in Prague were delayed by one year (2020 to 2021), the Commission enjoyed a four-year term rather than the usual three-year term. At the Congress, Gabriela Aurelio (Argentina), Françoise Damay (France), Dmitry Khalyavin (UK), and Noriki Terada (Japan) were elected as new voting members of the Commission, while Juan Rodriguez-Carvajal

(France) and Taku J. Sato (Japan) stepped down from the voting membership after many years of service. This reflects a net increase of two members, which increase was proposed by the Commission and approved by the GA. The voting membership of the Commission now includes Gabriela Aurelio (Argentina), Maxim Avdeev (Australia), Branton J. Campbell (USA, Chair), Francoise Damay (France), M. Teresa Fernandez-Diaz (France), Ovidiu Garlea (USA), Margarida Henriques (Czech Republic), Dmitry Khalyavin (UK), J. Manuel Perez-Mato (Spain), Noriki Terada (Japan), Andrew Wills (UK) and Oksana Zaharko (Switzerland).

Mois I. Aroyo (Spain), Javier Campo (Spain), Daniel B. Litvin (USA), Alexander N. Pirogov (Russia) and Wieslawa Sikora (Poland) continue to serve as consultants to the Commission, and are now joined by Taku J. Sato (Japan) and Juan Rodriguez-Carvajal (France), who were previously voting members, as well as three new participants: Sudhindra Rayaprol (India), Oscar Fabelo (France) and Bob Von Dreele (USA).

This diverse team of members and consultants provides international scientific leadership by (1) developing and maintaining standards, software, and other infrastructure for magnetic crystallography; (2) fostering magnetic structure research communities in every part of the world; (3) supporting the editorial and publication efforts of IUCr Journals; (4) encouraging high-quality magnetic structure content at research meetings around the world; and (5) by organizing workshops and schools for training the next generation of early-career scientists. We note that the consultants to the Commission greatly enhance its geographic reach, core expertise, coherent infrastructure development, and training capacity.

### *IUCr Congress Program in Prague*

Despite the obstacles presented by the SARS-CoV-2 pandemic, the IUCr Congress and General Assembly in Prague were held successfully in a hybrid format in August 2021. We express gratitude to the Congress for persevering and overcoming these challenges. When the Congress was delayed from August 2020 to August 2021, most micro-symposia and Keynote-speaker sessions went forward as originally planned, though there were a few minor changes in the session descriptions and Co-chairs. We note that in addition to the Commission's seven formally sponsored micro-symposia and one sponsored Keynote Lecture, four other sessions had strong magnetic crystallography themes. Participation was generally high in each of these sessions. We thank the Co-chairs of each session for attracting and selecting excellent speakers. Commission-nominated Keynote speaker Harold T. Stokes (USA) gave a highly engaging address entitled 'The Science of Symmetry Breaking: A Personal Journey'. We thank Oksana Zaharko, our representative to the Congress's International Program Committee, for their outstanding efforts to organize such a successful scientific program.

### *Standard and data development*

The anticipated article on the development of magnetic Hall symbols appeared in print in early 2021: *Extension of Hall*

*symbols of crystallographic space groups to magnetic space groups*, J. González-Platas, N.A. Katcho and J. Rodríguez-Carvajal, *J. Appl. Cryst.* (2021), **54**, 338–342. This effort was spearheaded by Commission member Juan Rodriguez-Carvajal.

During the summer, the Commission renewed the multi-year discussion of a new system of symbols for the 1651 three-dimensional magnetic space groups (MSGs). Based on the largely positive Commission feedback received on recent adjustments to the earlier 2018 proposal, B.J. Campbell, H.T. Stokes, J.M. Perez-Mato and J. Rodriguez-Carvajal finalized the details and prepared an article for publication: 'Introducing a unified magnetic space-group symbol'. The new unified (UNI) MSG symbol, which combines a modified Belov–Neronova–Smirnova (BNS) symbol with essential information from the Opechowski–Guccione (OG) symbol, is intended to (1) follow the Hermann–Mauguin conventions used in *International Tables for Crystallography*, (2) clearly convey the magnetic point group (MPG) of the MSG, (3) communicate the translational part of the time-reversal generator of each type-4 MSG, (4) separate the time-reversal from other generators for clarity, (5) distinguish each type-1 MSG from the corresponding non-magnetic space group, and (6) reveal the conventional lattice centering of both the MSG itself and the underlying non-magnetic space group. The paper appeared in print in January 2022 (*Acta Cryst. A* **78**, 99–106).

After three years of public beta testing within the ISOTROPY Software Suite, during which several problems were detected and resolved, Campbell and Stokes prepared a manuscript describing the exhaustive enumeration and tabulation of three-dimensional magnetic superspace groups with up to three independent modulations (over 325 000 groups). The MSSG symbols presented in this work are based on and compatible with the new UNI MSG symbols. This work is also expected to appear in print in 2022.

The Bilbao Crystallographic Server's MAGNDATA collection of magnetic structures has now expanded to include over 1700 magnetic structures, including 140 incommensurate magnetic structures. The Commission discussed possible approaches to turning this database into an exhaustive collection of magnetic structures. A recent feature was added to the MAGNDATA site, which allows users to submit magnetic structures themselves. It is hoped that this feature will help to distribute the workload of curating the required information.

### *Meetings*

Scientific meetings, schools, and workshops supported by the Commission include the following:

American Crystallographic Association (virtual sessions on 'Quantum Materials' and 'Magnetic Structure Determination'), 31 July – 5 August (lecturer: Branton Campbell).

Undergraduate Summer School on Magnetism and Magnetic Materials (virtual format), 8–15 August 2021, Florida State University, Tallahassee, Florida, USA (lecturer: Ovidiu Garlea).

IUCr Satellite Workshop on 'Aperiodic and Magnetic Structures for Beginners' (hybrid format), 12–13 August 2021,

Institute of Physics, Prague, Czech Republic (co-organizers and lecturers: Margarida Henriques, Vaclav Petricek, Juan Rodriguez-Carvajal, Manuel Perez-Mato, Bob Von Dreele, Branton Campbell and Harold Stokes).

25th IUCr Congress (hybrid format), 14–22 August 2021, Prague, Czech Republic (program developed and supported by the entire Commission).

School on ‘Representational Analysis of Magnetic Structures’ (RAMS 2021, hybrid format), 8–12 November 2021, University of Maryland, USA (lecturers: Margarida Henriques, Vaclav Petricek, Manuel Perez-Mato, Ovidiu Garlea, Andrew Wills, Bob Von Dreele and Branton Campbell).

**Branton J. Campbell**, Chair, and **J. Manuel Perez-Mato**, Secretary

#### 4.16. Commission on Mathematical and Theoretical Crystallography

The members of the MaThCryst Commission are V. A. Blatov (Russia), M. L. A. N. De Las Peñas (Co-chair, Philippines), J. Hadermann (Belgium), G. McColm (USA), H. B. Napolitano (Brazil), M. Nespolo (France), Wei Ren (People’s Republic of China), B. Stöger (Austria) and L. Suescun (Chair, Uruguay), and the consultants are M. I. Aroyo (Spain), J.-G. Eon (Brazil), E. Estévez Rams (Cuba), S. Hyde (Australia), V. Kurlin (UK), D. B. Litvin (USA), K. Momma (Japan), R. Oishi-Tomiyasu (Japan), D. Pradhan (India), D. Proserpio (Italy) and B. Souvignier (The Netherlands), and M. Fischer (Germany) and K. Stroz (Poland) joined as consultants after the IUCr Congress in Prague.

Communications among the members and consultants of the Commission took place via e-mail and Skype. These discussions were related to possible topics, venues and funding of future schools, workshops and satellite meetings, designation of a representative for MaThCryst on the International Programme Committee (IPC) of the 26th IUCr Congress and General Assembly and other outreach activities. Initial discussions of lists of speakers and Keynotes for the IUCr Congress in Melbourne were held by e-mail, moderated by the International Programme Committee representative for the Commission, Wei Ren.

The usual MaThCryst Commission activities were strongly affected by travel restrictions and the difficulty to organize in-person activities. The IUCr Congress held in Prague after the delay of 2020 concentrated much of the activities of Commission members. However, some activities took place during the year in both virtual and in-person modes:

M. I. Aroyo organized and co-chaired, with V. Kurlin (and P. Dlotko), the microsposium 25 ‘Computational Geometry, Topology and Symmetry Meet Material Science’ at the SIAM Conference on Mathematical Aspects of Materials Science, Bilbao, 17–28 May 2021, with 20 contributions distributed into 5 sessions in hybrid mode. M. I. Aroyo, V. Kurlin and M. L. A. N. De Las Peñas delivered invited talks.

Within the IUCr Congress in Prague, 14–22 August 2021:

M. L. A. N. De Las Peñas acted as IPC representative for MaThCryst, reviewing all bursary applications for the

Congress after the delay, and also acted as Keynote Moderator. They also co-authored two contributed talks ‘Coordinated colorings and their chromatic groups’ at MS-36 and ‘Layer groups associated with 3-way 3-fold isonemal fabrics’ at MS-65.

M. I. Aroyo co-chaired (with M. Henriques) MS-68, Symmetry Aspects of Magnetic Order and Magnetic Properties. They also delivered the invited talk ‘Symmetry database of International Tables online’ and were a co-author of the presentation ‘Crystallography online by the Bilbao Crystallographic Server: new computer tools for the study of layer and multilayer materials’. They also participated with G. de la Flor in the Software Fayre, presenting ‘Crystallography online by the Bilbao Crystallographic Server’.

V.A. Blatov delivered the invited talk ‘Perceiving zeolite self-assembly within the natural tiling mode’ at MS-65 and presented ‘Topological analysis with ToposPro and TopCryst’ at the Software Fayre.

J.-G. Eon delivered the invited talk ‘Combinatorial aspects of Löwenstein’s rule’ at MS-65.

J. Haderman co-chaired (with J. Sung) MS-48: Combination of X-rays and Electrons for Structure Characterization. They also delivered an invited talk ‘Uncovering hidden complexity in oxygen deficient perovskites’.

S. Hyde co-authored a selected talk ‘Behind the curve: Generating and analysing nets and tessellations on periodic minimal surfaces in their universal covering space’, delivered at MS-36.

V. Kurlin contributed two talks ‘Introduction to invariant-based machine learning for periodic crystals’ at SMS-3 and ‘A unique and continuous code of all periodic crystals’ at MS-65.

G. McColm co-chaired (with E. Miro) MS-112 Generalizations of Crystallographic Groups and Their Applications.

M. Nespolo co-authored the selected talk ‘Diffraction enhancement of symmetry and modular structures’ at MS-86.

R. Oishi-Tomiyasu delivered the selected talk ‘Global optimization of magnetic structure analysis by semidefinite relaxation method’ at MS-22.

B. Souvignier co-chaired (with M. Loyola) MS-65: Graphs, Tilings and Crystal Structures where V.A. Blatov and J.G. Eon were invited speakers and M. L. A. N. De Las Peñas and V. Kurlin gave contributed talks. They also co-authored the selected talk ‘Diffraction enhancement of symmetry and modular structures’ at MS-86.

B. Stöger co-chaired (with I. Pignatelli) MS-86: Modular Structure of Inorganic and Mineral Compounds.

L. Suescun presented a selected talk ‘Teaching crystallographic symmetry in Latin America. A 10-year review and perspectives’ at MS-96: Crystallography Schools to Promote Interdisciplinarity in Science.

M. Nespolo lectured in the five-day long course ‘Ninth basic course: Training course on symmetry and group theory’ at Sokendai Interdisciplinary Lecture Tsukuba, 13–17 September 2021. The course was suspended in 2020 and held in hybrid mode with the majority of participants online.

V. Kurlin organized the MACSMIN (Mathematics and Computer Science for Materials Innovation) virtual confer-

ence, Liverpool, 15–17 September 2021. V. Kurlin, B. Souvignier and M.I. Aroyo delivered talks. (<http://kurlin.org/macsmmin.php#2021>.)

M.I. Aroyo additionally delivered invited talks on the Bilbao Crystallographic Server at the Fall meeting of the European MRS and at the On-line Workshop Computational Methods in Materials Science: Fundamentals and Applications CMMS-2021, Warsaw, Poland in September.

The Commission changed its membership from 10 members and the Chair to 8 members and the Chair during the 25th General Assembly. During the year the Commission discussed an internal rule to select future Commission members. A preliminary conclusion to the discussion, which should become an internal rule before the next IUCr Congress, is that new members should be appointed as consultants for at least one triennium before joining as members. During that triennium they must show some degree of activity within the goals of the Commission that suggests that their membership will be productive.

Some members of the MaThCryst Commission have acted as Editors or reviewers of IUCr publications and journals:

M.I. Aroyo performed activities as Editor of Volume A, the Teaching Edition, the Symmetry Database and Teaching Edition of the Symmetry Database of *International Tables for Crystallography*, and is also a Co-editor for *Acta Crystallographica Section A*.

M. Nespolo is Book Review Editor for IUCr Journals.

After the 2nd MACSMIN conference a lively discussion has been ongoing within the Commission about lattice classifications and different approaches to the solution to the question 'Are two lattices equal?', which arises frequently during crystal structure analysis using large volumes of crystallographic data sets. This issue will be treated in one of the proposed micro-symposia for the 26th IUCr Congress in Melbourne and discussions will continue throughout 2022 in the MaThCryst-supported MIF++ Network Seminars organized by V. Kurlin. Hamilton Napolitano has proposed Universidade Federal de Goias, GO, Brazil, as the host of the ISFC-2022, 7th MathCryst School in Latin America, a very welcome proposal to re-start the series of schools that had run continuously since 2007 and was interrupted by the events of 2020. Discussions on the program and organization details developed during the year and will crystallize in late 2022 or early 2023.

The Commission's web page (<https://crm2.univ-lorraine.fr/mathcryst/index.php>) is maintained and frequently updated by M. Nespolo.

**Leopoldo Suescun**, Chair

#### 4.17. Commission on Neutron Scattering

The Commission (the CNS) promotes the use of neutron scattering by encouraging the publication of information on the capabilities of neutron sources and instrumentation and by supporting symposia, schools and workshops that educate researchers on the unique information that can be provided by neutron scattering. Several members of the Commission are

actively involved in developing neutron sources and new neutron scattering technologies and methods.

Operation of the major neutron facilities has continued except for temporary closures and/or suspension for user operation in some facilities due to COVID-19; however, one should note the great efforts made to maintain activities by the staff, especially at the ILL, replacing the users. In addition, remote experiments and rapid-access programmes were widely introduced in many facilities during the COVID-19 pandemic.

The construction of the European Spallation Neutron Source (ESS) in Sweden is progressing and on track to deliver neutrons to eight instruments by 2025. Although the Orphée reactor at the Laboratoire Léon Brillouin (LLB) in France was shut down, the LLB is still the neutron scattering centre for French users involved in different outstations at the ILL, PSI or building five instruments at the ESS. To face these challenges, a League of advanced European Neutron Sources, LENS, was created: this is a not-for-profit consortium working to promote cooperation between European-level neutron infrastructure providers offering transnational user programmes to external researchers. It should also be noted that numerous groups have been working on alternative sources to compensate for the loss of neutrons for research in Europe, an example being the meetings of the Jülich Centre for Neutron Scattering (JCNS) concerning the potential technical design of a so-called High Brilliant Source (HBS) and suitable instrumentation.

The Spallation Neutron Source (SNS) in the USA continued operation at 1.4 MW providing more than 4500 neutron production hours annually. Progress continues on the Proton Power Upgrade (PPU) project for the SNS, which will be complete in 2025. The PPU project will double the power capability of the SNS accelerator from 1.4 to 2.8 MW, to facilitate new types of experiments and discoveries. The High Flux Isotope Reactor (HFIR) in the USA continued operation at 85 MW, providing more than 3900 neutron production hours annually.

J-PARC MLF in Japan also continued operating with 700 kW beam power, and the beam power will be upgraded step by step every year. The Japanese Research reactor (JRR-3) restarted operation from February 2021 after ten years of shutdown. The beam power of the Chinese Spallation Neutron Source (CSNS) reached 100 kW and a user programme was started.

Accelerator-driven neutron sources for neutron scattering applications are running, under discussion or under construction around the world. A meeting was held virtually at Rikken (Japan) regrouping all compact accelerator-based neutron sources (CANS) in December 2021, with another at the Union for Compact Accelerator-driven Neutron Sources 9 (UCANS9) meeting in March 2022. In Europe there are several projects to develop and build high-current accelerator-based neutron sources (HiCANS), and an association called ELENA was created, where these projects are cooperating.

Our Commission members were also involved in organizing several meetings, not only for neutron but also for quantum-



beam (synchrotron, neutron and ion radiation *etc.*) joint use, that took place in 2021, including various annual meetings of regional crystallographic associations, Association Française de Cristallographie in Grenoble, France, 29 June – 2 July 2021, and the 7th Conference on Neutron Scattering (CNS-2021) at Bhabha Atomic Research Centre, India, 25 – 27 November 2021 (in hybrid mode).

Several neutron schools at many facilities and crystallographic seminars are supported by Commission members each year in many countries or regions. In 2021, some of these schools and seminars were held in virtual classrooms. At J-PARC, the 5th Neutron and Muon School was held virtually, including a virtual experiment, 6–9 December, with 95 students from 14 countries; similarly with the HERCULES course held in Grenoble in March 2021. Some schools were on site, such as the FANS at the ILL in October 2021.

Commission members were involved in planning activities for several important neutron-related conferences and schools in 2022. Owing to the still rampant COVID-19, some conferences, meetings and schools will be held in virtual classrooms.

**Toru Ishigaki**, Chair

#### 4.18. Commission on NMR Crystallography and Related Methods

In addition to participation at the triennial IUCr Congresses, the Commission on NMR Crystallography and Related Methods works towards several outreach objectives. Examples of such activities include coordination and sponsorship of themed sessions on NMR crystallography at annual meetings of the American Crystallographic Association and the SMARTER conferences. As the global COVID-19 pandemic continued through 2021, many of these activities have remained on hold. The highlight of 2021 for the Commission was the success of the hybrid Twenty-Fifth Congress and General Assembly of the International Union of Crystallography, held jointly in Prague and online.

The Commission led two microsymbiosia, one entitled ‘Polymorphism and structural transformation of organic crystals from synthesis to characterization’ and one entitled ‘New methods and strategies in NMR crystallography – in honour of Francis Taulelle’. In addition, the Commission supported two further microsymbiosia, namely those on ‘Porous framework materials for gas adsorption/separation’ and ‘Spectroscopy applied to electrochemistry: operando studies’. Further, the Commission is proud to have proposed one of the Plenary speakers, Professor Clare Grey of the University of Cambridge, who spoke on ‘In situ and ex situ studies of battery materials with magnetic resonance and diffraction methods’.

In addition to pandemic related obstacles, the founding Chair of the Commission, Professor Francis Taulelle, passed away in early 2021. This prompted a renewal of the Commission membership, with Professor David Bryce taking over the Chair role of from interim Chair Professor Manish Mehta in 2021. New members and consultants were also

rotated onto the Commission with particular emphasis on diversity and broad representation of the international community. [Members: D. Bryce (Chair, Canada), S. Brown (UK), A. Commoti (Italy), Y. Khimyak (UK), M. Leskes (Israel), P.K. Madhu (India), Y. Nishiyama (Japan), T. Polenova (USA) and J. Senker (Germany). Consultants: A. Gippius (Russia), M.A. Mehta (USA), J. Rocha (Portugal) and R.E. Wasylishen (Canada).]

Looking forward, the Commission has begun active planning for the activities of the next IUCr Congress to be held in Melbourne in 2023. Commission member Professor Yaroslav Khimyak is serving as our representative on the International Program Committee. As the pandemic continues to ease and we return to in-person events, the Commission plans to revitalize links between the NMR and diffraction communities through conferences, workshops, and other outreach activities.

**David Bryce**, Chair

#### 4.19. Commission on Powder Diffraction

The COVID-19 pandemic continued to impact significantly on the activities of and planning by the Commission for Powder Diffraction (the CPD). This has resulted in the postponement and in some cases cancellation of meetings and workshops while members focused on more immediate crises impacting on them personally and professionally. A prime example of a postponed meeting was EPDIC17, which will finally take place 31 May to 3 June as an in-person event after a two-year postponement.

The CPD did, however, support the following meetings: the 7th European Crystallography School, the 18th International Conference on X-ray Absorption Fine Structure, the Virtual Pan African Conference on Crystallography (ePCCr), the IV LACA School of Crystallography – Phase Identification and Microstructural Characterization of Materials using X-ray Powder Diffraction Techniques, and To.Sca.Land 4.0: Total Scattering in Al Andalus.

Following a successful program at the Prague Congress and General Assembly, focus has shifted to the 2023 Melbourne Congress and General Assembly. For this meeting the CPD successfully negotiated for two representatives on the IPC, and will be represented by Angus Wilkinson (USA) and Antonia Neels (Swiss) at the upcoming IPC meeting.

The CPD is also pleased to confirm that the 59th International School of Crystallography in Erice will be devoted to powder diffraction and has been scheduled for 31 May to 8 June 2024. The 3rd Southern African Powder Diffraction Conference and Workshop is also in the early planning stages and scheduled for 16–21 April 2023 in Namibia.

It has proven rather challenging to make progress with projects. This is mostly due to limited resources and the already high demands on their time from their primary employers experienced by most members. It might be worthwhile approaching some retired ex-CPD members for this, possibly as commissioned work for which funding can be sought.

Ongoing CPD projects include:

(i) *Recommended practice and publication guidelines*. Most members are concerned about the poor quality of data published in many journals and the fact that this is generally exacerbated by poor reporting and/or poor interpretation of the data.

(ii) *Powder CIF project*. In the last year this has received considerable attention in collaboration with a number of IUCr staff from Chester, with a three key areas of attention.

(a) Development a tool for ready viewing and analysis of, particularly, data sets containing multiple scans (as would, for example, result from variable-temperature or *in situ* studies). This was largely driven by Matthew Rowles, and *pdCIFPlotter* is now being distributed along with a set of macros for use with *Topas* to produce the pdCIF files. A paper detailing *pdCIF-plotter* has been submitted to *J. Appl. Cryst.* The intention next is to convince authors of other powder programs to also facilitate the production of pdCIFs, and to subsequently use this to improve the quality of published results based on powder data.

(b) Initial discussions have taken place to make the online *checkCIF* algorithms more compatible with standard powder practices and methods.

(c) The Commission has also been part of a task team to look at making powder data more machine readable. A paper on this has been submitted to *Acta Cryst. A*.

**Dave Billing**, Chair

## 4.20. Commission on Quantum Crystallography

In 2021 the Commission on Quantum Crystallography (QCr) slowly returned to its usual activities, after perturbations caused by the COVID-19 pandemic.

In August 2021, the IUCr Congress in Prague took place, in which the QCr community participated very actively. The QCr field was represented by two Keynote Lectures given by Dylan Jayatilaka (Quantum Crystallography: Past, Present, and Future) and Piero Macchi (Quantum Crystallography and Spintronic Materials). The lectures were among the most highly attended at the Congress. Six microsymbiosia were organized by the Commission, alone or with the cooperation of other Commissions. All microsymbiosia had many participants, joining online or from on site. During the Congress an open QCr Commission meeting was also organized, at which decisions about future conferences, lecture series and schools took place. The topics of QCr software development and maintenance as well as the QCr CIF dictionary expansion were discussed.

In September 2021, Piero Macchi and Alessandro Genoni organized the CECAM workshop entitled 'Second Discussion Meeting on Quantum Crystallography: Expectations and Reality', which followed the first discussion meeting on quantum crystallography that took place in Nancy (France) in June 2017. The idea was to discuss the state of the art and possible future developments in the QCr field after the first CECAM workshop. The workshop was organized online and thanks to that a large number of participants were allowed.

In December 2021, the Distinguished Lectures on Quantum Crystallography and Complementary Fields were launched online. The series is organized jointly by the QCr Commission and the European Crystallographic Association SIG-2 on Quantum Crystallography, with the support of the Department of Chemistry of the University of Warsaw (Poland) and the Crystallography Committee of the Polish Academy of Sciences. Since then, two lectures have been broadcasted each month, one given by a member of QCr community, another by a speaker representing a complementary field. The series is a great success, with more than 300 registered participants from all over the world, and 90–140 people attending each lecture.

In 2021 the Commission recommended that the IUCr support the 9th International Charge Density Meeting to be organized by Professor Jacob Overgaard and Professor Anders O. Madsen in Aarhus, Denmark, 13–17 June 2022. The Commission has also strongly supported the 'An integrated 'workbench' for Quantum Crystallography' application submitted to the UK Engineering and Physical Research Council by Simon Coles and Horst Puschmann.

**P. Dominiak**, Chair

## 4.21. Commission on Small-Angle Scattering

The following report was prepared by Jan Ilavsky, SAS Commission Chair, together with members Emmanuel Kentzinger, Kristina Djinovic Carugo, Elliot Gilbert, Duncan McGillivray, Eleonora Shtykova, Masaaki Sugiyama and Florian Edouard P. Meneau, and consultants Andrew Allen, David Babonneau, Javier Pérez, Daniel Clemens, Pete Jemian, Jill Trehwella, Dmitri Svergun, U-Ser Jeng and Iris Torriani.

For 2021, the business of the SAS Commission (CSAS) was conducted mostly via e-mail or online meetings, as usual personal meetings at national and international conferences were not possible due to the COVID-19 pandemic.

CSAS members are providing active support to the SAS 2021 conference, which was postponed to September 2022. Several CSAS members participate as committee members and help in local conference outreach.

The pandemic restricted many activities for all CSAS members and consultants. Nevertheless, what follows is a summary of highlights of activities for 2021.

### *Commission activities, meeting, and communication*

U-Ser Jeng served as CSAS Chair until the 25th IUCr Congress, and handled the transition to the new Chair and the addition of two new CSAS members, Dr Florian Edouard P. Meneau (Brazil) and Dr Emanuel Kentzinger (Germany), and one new consultant, Dr David Babonneau. They also had a meeting with the IUCr Executive Committee (EC) to discuss the details of the changes and provided suggestions from CSAS to the EC. U-Ser communicated with the CSAS members and consultants for promotion and supporting of 6 SAS microsymbiosia for the 25th IUCr Congress, and after the Congress started serving as a representative delegate from Taiwan at the IUCr General Assembly.

Jan Ilavsky became Chair of CSAS at the 25th IUCr Congress in Prague, and organized an online meeting of CSAS to establish dialogue and communications.

Andrew Allen continued to serve as CSAS representative, throughout 2020 and 2021, on the International Programme Committee (IPC) for the postponed IUCr Congress in Prague, a hybrid conference with only limited actual participation in Prague, Czech Republic, and a virtual conference for all others. Nevertheless, most of the previously negotiated SAS-related microsymbiosia and the SAS-related Keynote talk proceeded as part of the IUCr Congress programme. Andrew continues to serve as a member of the new IPC for IUCr 2023 as IUCr Journals Editor-in-chief.

M. Sugiyama collaborated with Dr Frank Gabel at Institut de Biologie Structurale, France, and organized a micro-symposium ‘Solution Scattering and Combined Techniques for Complex Biological Systems, Including Component Dynamics’ at the 25th IUCr Congress.

Florian Meneau is Chair of the upcoming XVIII International Small-Angle Scattering Conference (SAS2022), and worked on the postponement of the SAS-2021 triennial conference at Campinas, Brazil, to 2022 (now rescheduled to 11–16 September 2022), to avoid competing with the rescheduled IUCr Congress. Florian applied to the IUCr as well as Brazilian funding agencies CAPES and FAPESP for financial support for students to participate at SAS2022.

#### *Educational activities*

Andrew Allen worked with IUCr Editorial Office staff in planning and execution of IUCr Journals Author Workshops and other activities for the Congress. Both a virtual workshop for prospective and existing IUCr journal authors, ‘From Data to Publication’, and a virtual Journals Commission meeting for all IUCr Journal Editors were held during the Congress.

#### *Community-building activities*

Andrew Allen served as Editor-in-chief of IUCr Journals. As such, Andrew continues to encourage negotiations between the SAS 2022 Conference organization and IUCr Journals for developing an open-access Special Issue of the *Journal of Applied Crystallography* to be associated with the conference.

Jan Ilavsky continues to serve as Co-editor for the *Journal of Applied Crystallography*.

Elliot Gilbert continues to serve as Co-editor for the *Journal of Applied Crystallography*, and is also guest Co-editor for an upcoming Special Issue of the *Journal of Applied Crystallography* dedicated to ‘Magnetic small-angle neutron scattering – from nanoscale magnetism to long-range magnetic structures’. Elliot delivered an invited talk at the 25th IUCr Congress, ‘Characterizing Food Materials and the Case for Extended q Scattering’.

D. Svergun continues as a Co-editor of the *Journal of Applied Crystallography*, and U-Ser Jeng continues to serve as a Co-editor for the *Journal of Synchrotron Radiation*.

#### *Consultant activities*

Andrew Allen continued to provide informal input for drafts for ISO standards on the use of small-angle scattering, specifically SAXS for particle characterization. A revision of

ISO 17867: 2020 Particle size analysis – small-angle scattering was completed for the existing ISO standard on particle size determination using SAXS and issued in early 2021. Significant progress continued in 2021 on the new ISO standard (ISO 20804) being developed to cover surface area measurement using SAXS methods. In both cases, critical aspects of characterizing particle size distributions (not just mean size), and particle shape, are now being incorporated into the new standard as key issues in relating surface area measurements (using Porod scattering *etc.*) to particle size and volume fraction.

Jill Trehwella continues to serve as a member of the Protein Data Bank (PDB) Advisory Committee, providing expert input on small-angle scattering (SAS) and its role in integrative/hybrid structure determination. In this capacity Jill has advised the developers of the PDB’s prototype integrative methods archive PDB-Dev on metrics for SAS data quality and model validation that will be displayed with deposited structures.

#### *International activity*

David Babonneau co-chaired the microsymposium *Integrative methodologies for novel thin film structures* (MS180) at the 25th IUCr Congress in Prague, Czech Republic, with B. Krause (Germany), and Jan Ilavsky co-chaired MS75 *Small- and wide-angle scattering for industrial materials far from equilibrium*.

#### *Technical activities*

Andrew Allen continued to provide technical support to users of the NIST Standard Reference Material (SRM) SAXS Intensity Standard: NIST SRM 3600, and continues to encourage development of a SAXD *q*-Calibration Standard NIST SRM. Andrew is also involved in current revision of gold nanoparticle suspension NIST Reference Materials, RM8012 and RM8013, partly based on SAXS measurements.

Eleonora Shtykova (with Maxim Petoukhov and Petr Konarev) participated in the further development of the software package *ATSAS*: the latest release of the *ATSAS* program suite is available for academic users at <https://www.embl-hamburg.de/biosaxs/software.html>.

Jan Ilavsky maintains the software packages *Irena* and *Nika* used widely by the materials science SAS community for data reduction and analysis.

D. Svergun’s group continued to maintain and curate the Small Angle Scattering Biological Data Bank (<https://www.sasbdb.org>; main curators A. Kikhney and C. Jeffries), which presently contains over 2600 data sets and over 3700 models. The *ATSAS* program package (currently at version number 3.0.5) has over 16 000 users from over 50 countries.

Jill Trehwella reports that the article *2017 Publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update* by Trehwella *et al.* in *Acta Cryst. Section D* continues to attract strong readership and is now to be referenced by IUCr biology journals in the notes for authors submitting SAS-derived models, who now will be advised they must submit their data to the SASBDB and use the recommended tables for presentation of methods and results. As Chair of the PDB SASvtf and a

consultant on CSAS, Jill is continuing as the lead coordinator for the initiative that aims to generate a set of SAS data sets that can be used to benchmark different approaches to predicting SAS profiles from atomic coordinates (see <https://sas.wwpdb.org/?q=node/25> for full details and participants). The effort included CSAS consultants Javier Pérez and Dmitri Svergun, and has grown to include 49 structural biology and SAS experts from across Europe, Asia and the Americas. During 2021, data analysis continued to progress for the 150 SAXS data sets and more than 70 SANS data sets submitted from 12 SAXS facilities and 4 SANS facilities, including SEC-SAXS and batch SAXS, SEC-SANS and batch SANS in H<sub>2</sub>O and D<sub>2</sub>O. A new tool for data combining was developed to facilitate finding the best consensus results for each protein studied. A draft paper for *Acta Cryst. Section D* is in the final stages of editing for distribution to participants, and will be accompanied by deposition of data for five proteins as suitable for benchmarking methods for SAS profile prediction.

Jan Ilavsky, Chair

## 4.22. Commission on Structural Chemistry

The Commission on Structural Chemistry (the CSC) encompasses a wide range of topics in the field of crystallography. There are extensive overlaps with other Commissions, including the Commissions on Inorganic and Mineral Structures, Powder Diffraction, and Crystallographic Teaching, as well as with important external bodies such as the Cambridge Crystallographic Data Centre (CCDC).

The Commission last met in person at the 2017 Hyderabad Congress and there agreed to focus on (i) support for appropriate crystallographic conferences and schools, in particular those that aim to expand crystallography to under-represented regions such as South America and Africa; (ii) support for IUCr Journals, through encouraging submission of excellent scientific results to *IUCrJ* and other journals; and (iii) building relations with other Commissions and external bodies such as IUPAC and the CCDC.

The membership of the Commission was renewed in 2021. The members of the Commission (until 2023) are: Rahul Banerjee (India), Susan Bourne (South Africa, Chair), Marijana Đjaković (Croatia), Alison Edwards (Australia), Javier Ellena (Brazil), Katherina Fromm (Switzerland), Jun Harada (Japan), Len MacGillivray (USA), Andy Maloney (CCDC, UK), Pance Naumov (UAE) and Shie-Ming Peng (Taipei).

The Commission is fortunate to have a number of consultants who provide guidance and continuity. These are Christer Aakeröy (USA), Alessia Bacchi (Italy), Maria Bernini (Argentina), Agata Bialonska (Poland), Nadeshda Bolotina (Russia), Petra Bombicz (Hungary), Alexander Briceño (Venezuela), Ilia Guzei (USA) and Chris Ling (Australia; liaison with the Commission on Inorganic and Mineral Structures).

The Commission expresses its thanks to Christian Lehmann (Germany) and Giuseppe Resnati (Italy), who stepped down

after each serving three terms on the Commission, and to Patrick Mercier (Canada) and Stuart Batten (Australia) who had served as consultants.

In 2021, the CSC lent support to the following conferences and schools, which draw on crystallographers in the structural chemistry sphere:

International School of Crystallography: Diffuse Scattering: The Crystallography of Dynamics, Defects, and Disorder, Erice, Italy, June 2022.

7th European Crystallography School (ECS), Lisbon, Portugal, July 2022.

Two satellite meetings to ECM33: High Pressure Crystallography, and Chirality in Crystals, Lège-Cap Ferret, France, August 2022.

Symposium in memory of Marilyn Olmstead at the ACS meeting, Chicago, USA, August 2022.

5th International Symposium on Halogen Bonding (ISXB5), Kisarazu, Japan, November 2022.

The CSC members interrogated the degree to which structural chemistry was represented as a science, rather than simply a tool, at each conference. Aspects such as support for students or early-career researchers were taken into account. The diversity (gender, geographical distribution) of speakers was also identified as an important criterion for consideration of future applications for support. These factors play a key role in the degree of support expressed to the IUCr's Subcommittee on the Union Calendar.

As in 2020, organizing committees had to consider the COVID-19 pandemic in their planning. In most cases, the conferences are planned to be in person, often with a hybrid option. In almost all cases, organizers have a plan to move the conference online should local or international restrictions prevent delegates from travelling.

A successful hybrid IUCr Congress was held in Prague, Czech Republic, in August 2021. The CSC was well represented in terms of subject matter (Keynote Lectures, microsymbiosia) and participants (delegates and session Chairs).

Planning is well underway for the next IUCr Congress in 2023 in Melbourne, Australia. The CSC representatives on the International Programme Committee, Delia Haynes, Tomoji Ozeki, and Christian Lehmann, have circulated an extensive list of suggested microsymbiosia and Keynote speakers, including some in collaboration with several other Commissions. These will be discussed and refined during the IPC meeting in April 2022. We look forward to a strong structural chemistry programme at the 26th IUCr Congress in Melbourne.

Susan Bourne, Chair

## 4.23. Commission on Synchrotron and XFEL Radiation

The mission of the Commission on Synchrotron and XFEL Radiation (SXR) is to promote access and awareness of crystallographers worldwide to the world's synchrotron radiation (SR) and X-ray free-electron laser (XFEL) facilities. To this end, the Commission promotes the development of



crystallographic instrumentation, technology and standards, and the synergies between storage-ring-based and LINAC-based next-generation XFEL sources. The bulk of the Commission's work is carried out via e-mail. Since Autumn 2021, we have been having two online meetings (Autumn and Spring) per year.

#### *Synchrotron radiation and free-electron laser facilities*

Following the beginning of operation of the first '4th generation' storage ring, MAX IV in Sweden, many synchrotron facilities have been planning to upgrade or build new rings. For example, the ESRF completed a major upgrade of its accelerator in 2020 and beamlines have been upgraded in 2021. The APS upgrade was approved and replacement of the ring will start in 2022. Following in the footsteps of these two hard X-ray facilities, Spring-8 is also planning significant upgrade programmes based on these new designs. In addition, SIRIUS, the 4th-generation Brazilian facility, has most of its beamlines under commissioning and the 6 GeV High Energy Photon Source (HEPS) is being built near Beijing, China. Many other facilities have plans to adapt the new high-brightness designs.

There are now 5 hard X-ray FELs open to users worldwide: the European XFEL in Germany, SACLA in Japan, PAL-XFEL in South Korea, SwissFEL in Switzerland and the LCLS in the USA. The first hard X-ray FEL based on superconducting accelerator technology, the European XFEL, started operation in 2017. A major upgrade is ongoing for the LCLS with the installation of a 4 GeV continuous wave (cw) mode superconducting accelerator and a new suite of soft X-ray instruments. SwissFEL is continuing to increase the instrument portfolio. In addition, with SHINE a new 8 GeV cw-mode superconducting accelerator FEL facility is under construction in Shanghai (China).

#### *Commission membership*

The current members and consultants are as follows. Members (with year appointed): M.A.G. Aranda (Spain) (2011), Chair; T. Tschentscher (Germany) (2014); E. Granado (Brazil) (2014); T. Hatsui (Japan) (2017); M. Kozak (Poland) (2017); S. Ramaswamy (India/USA) (2017); Lisa Keefe (USA) (2021); Shin-Ichi Adachi (Japan) (2021); Esna du Plessis (South Africa) (2021); and Aina Cohen (USA) (2021). Consultants: P. Grochulski (Canada), former Chair; R. Garrett (Australia) previous Chair; D. Fritz (USA); M. K. Sanyal (India); N. Zatsepin (Australia); J. Smith (USA); Allen M. Orville (UK); and Martín E. Saleta (Argentina).

#### *Supported meetings, schools and workshops*

During 2021 the COVID-19 pandemic continued to have an impact on these events. The Commission provided letters of support and endorsement for the following meetings in 2021:

18th International Conference on X-ray Absorption Fine Structure, XAFS 2022. Initially scheduled for July 2021, this will take place in July 2022 in Sydney (Australia).

15th edition of the 'International School on Synchrotron Radiation, Fundamentals, Methods and Applications'. This will take place in September 2022 in Trieste (Italy). It is being organized by the Italian Synchrotron Radiation Society in collaboration with Elettra.

16th International Conference on the Physics of Non-Crystalline Solids, PNCS16. This will take place in July 2022 in Canterbury, Kent, UK.

In general, the Commission has strongly supported IUCr sponsorship for the purpose of assisting attendance by young researchers and scientists from developing countries.

DESY and the European XFEL were the hosts of the 14th International Conference on Synchrotron Radiation Instrumentation, planned to be held at the end of August in Hamburg, Germany. Owing to the pandemic situation and the desire to organize an in-person meeting allowing deeper exchange of information, the International Advisory Committee decided in the spring to shift the meeting to 2022. Furthermore, the European XFEL and DESY organized a regular virtual seminar series from January 2021 which focused on new developments of broad interest at the hard X-ray FEL facilities. Speakers are from the five operational facilities LCLS, SACLA, PAL-XFEL, the European XFEL and SwissFEL, and as well from SHINE, which is under construction. The meeting is open to any interested audience (contact Th. Tschentscher, European XFEL).

#### *Activities of members and consultants*

The members of the Commission are active in key synchrotron and crystallography communities and conferences. For example:

Miguel A. G. Aranda was elected as a member of the Scientific Advisory Council of ELETTRA in 2021, to start January 2022. Miguel also gave an invited (online) talk: 'Analysis of building materials by synchrotron X-ray imaging' at the Spanish Crystallographic Association Meeting, January 2021, and an invited (online) seminar: 'Synchrotron Radiation and Building Materials: Adapting the techniques to relevant samples and not the other way around' at the ALBA-II set of seminars, in May 2021.

Martín E. Saleta was a member of the Scientific Committee of the Argentinean Crystallographic Association Meeting (2021 and 2022), and gave an invited (online) talk: 'Study of magnetic oxides and semiconductors using synchrotron techniques' at the IX AACr Workshop: Synchrotron Light Radiation in November 2021.

Thomas Tschentscher was a Co-chair of the SRI 2021 local organizing committee.

#### *Asia Oceania Forum for Synchrotron Radiation Research*

The Asia Oceania Forum for Synchrotron Radiation Research (AOFSRR) is an international network of synchrotron and XFEL light source facilities and user organizations in the Asia Oceania region. Commission consultant Richard Garrett is Secretary-Treasurer of the Forum. The Forum holds an annual week-long school for graduate students and early-career researchers, which rotates between the AOFSRR members, and an annual workshop. In 2019 the AOFSRR announced that it would establish an Asia Oceania Synchrotron Radiation Instrumentation conference series (AO-SRI), to be held every three years in between the International Conferences on Synchrotron Radiation Instrumentation (SRIs).

Owing to COVID-19 and the restrictions on international travel, all in-person AOFSSR events planned for 2020 and 2021 were postponed. The 2020 AOFSSR Synchrotron School, to be hosted by the Synchrotron Light Research Institute, Thailand, is now planned for October 2022. The first AO-SRI Conference will be held in Sendai, Japan, chaired by the Photon Science Innovation Center and hosted by Tohoku University International Center for SR Innovation Smart. The conference, originally planned for late 2020, has been postponed and is now planned for November 2022. The International Particle Accelerator Conference IPAC'22 supported by the AOFSSR Council is scheduled to be held on site in Bangkok, Thailand in June 2022.

Miguel A. G. Aranda, Chair

#### 4.24. Commission on XAFS

##### *Members and duties*

During the XXV General Assembly and Congress of the International Union of Crystallography in Prague in August 2021, the changes proposed for the membership of the Commission on XAFS (CXAFS) were approved. As has been the case previously, each of the members has a specific portfolio that they are responsible for. This has worked very well until now, and everybody contributes to the activities of the Commission.

The approved membership and portfolios are: Sofia Diaz-Moreno (UK), Chair, Liaison with IXAS (until 2022), Coordinator of next Q2XAFS meeting; Guiliiana Aquilanti (Italy), Secretary, Liaison with the International Program Committee (Melbourne 2023); Valerie Briois (France), Secretary, CXAFS website; Hitoshi Abe (Japan), Working Group on Databases, Coordinator of Summary from Japan XAFS Society, Liaison with IXAS (after 2022); Dibyendu Bhattacharya (India), IUCr Melbourne 2023 Congress XAS Workshop; Steve M. Heald (USA), Liaison with *International Tables of Crystallography* and IUCr Journals; Rene Loredó Portales (Mexico) and Gloria Subias-Peruga (Spain), Coordinators of funding support from the Sub-committee on the Union Calendar; Chanh Q. Tran (Australia), Local XAS representative for the IUCr Congress in Melbourne 2023, including XAFS workshop and Q2XAFS conference; Edmund Welter (Germany), Coordinator of round-robin activity, Coordinator of next Q2XAFS meeting; and Anna Wolska (Poland), IUCr Online Dictionary (for XAFS terminology), Liaison to *International Tables*.

Consultants: Chris Chantler (Australia), Federico Boscherini (Italy), Richard Strange (UK), Farideh Jalilehvand (Canada), Matt Newville (USA) and Bruce Bunker (USA).

The Commission meets once a month. Subjects such as requests for support for events, organization of workshops and conferences, CXAFS web-page contents, *etc.* are regularly discussed.

##### *International Tables for Crystallography Volume I*

All three Editors have been working diligently towards the volume, and good progress has been made. There are now 45

chapters typeset and available online (<https://it.iucr.org/I/>). Of the ten sections that form the volume, Sections 2, 7, 8, 9 and 10 are very close to completion, while Sections 3, 4 and 5 are near completion. Section 1 is the summary, and it will be addressed after all the sections are completed.

We expect to be in a position so we can advertise the volume at the International XAFS conference in Sydney (Australia) in July 2022. It will be a great achievement if the volume is ready for the 26th General Assembly and Congress of the International Union of Crystallography in Melbourne (August 2023).

*CXAFS support for the XXV General Assembly and Congress of the International Union of Crystallography*

The Commission was very active during the XXV Congress in Prague in 2021.

Most of the microsymbiosia supported and organized by our Commission, alone or in collaboration with other Commissions, were very successful, and two of them are in the top 25 by number of views. The 'Catalysis: functionalized materials studied by XRD and XAFS', the 'Advanced methods for analysis of XAFS and crystallographic data' and the 'Disordered materials: spectroscopic and scattering techniques' microsymbiosia were very well received, with a large number of abstracts received (between 46 and 17). The last one was so popular that it had to be divided into two separated sessions.

##### *CXAFS support for other meetings*

CXAFS provided support during the organization of the International Conference on XAFS held in Sydney in 2021 (a virtual event).

Ongoing support is being provided by many of the members of the Commission for the hybrid event organized for 2022. CXAFS has also led the request for financial support and endorsement from the IUCr for this event, together with the Commission on Powder Diffraction and the Commission on Synchrotron and XFEL Radiation.

CXAFS has formally endorsed the request for financial support and sponsorship from the IUCr for the 16th International Conference on the Physics of Non-Crystalline Solids to be held in July 2022 in Canterbury (UK).

CXAFS has also formally endorsed the request for financial support and sponsorship from the IUCr for the 15th edition of the International School on Synchrotron Radiation, Fundamentals, Methods and Applications to be held in September 2022 in Trieste (Italy). The event was also endorsed by the Commission on Synchrotron and XFEL Radiation.

*Preparations for the Q2XAFS conference and the XAS workshop as part of the XXVI Congress*

As part of the XXVI IUCr Congress, the Commission on XAFS is organizing a one-day XAS workshop with international invited tutors. In addition, and as a satellite of the main event, CXAFS and the International XAS Society are working together to organize the Q2XAFS conference.

Sofia Diaz-Moreno, Chair, and Valérie Briois and Guiliiana Aquilanti, Secretaries

## 5. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support, and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 2021 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those that were held in 2021 are listed at the beginning of this Report of the Executive Committee. Those that were approved in 2021 but are due to be held in 2022 are listed below. (It should be noted that this list, shorter in length than usual, does not include those meetings that were approved but subsequently postponed or cancelled.)

Tunisian Powder Diffraction School, Monastir (Palais des Sciences de Monastir), 21–24 January 2022.

56th School 'Crystallography under extreme conditions – the future is bright and very compressed', Erice, Italy, 3–11 June 2022.

57th School 'Diffuse Scattering: the crystallography of dynamics, defects, and disorder', Erice, Italy, 3–11 June 2022.

International Conference on the Chemistry of the Organic Solid State (ICCOSS XXV), Ohrid, Macedonia, 3–9 July 2022.

Organizers of meetings wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the meeting, writing to the Chair of the Sub-committee. For up-to-date contact information, application procedures and rules, see <https://www.iucr.org/iucr/sponsorship/meetings.html>.

Requests from satellite meetings may be submitted, and possible financial support requested, separately or through the Organizing Committee of the main meeting.

Meetings (other than satellite meetings) scheduled to be held within one month before or after an IUCr Congress will not be considered for sponsorship. For any meetings scheduled to be held between one and two months before or after a Congress, the application for sponsorship will be sent to the Chair of the Congress Programme Committee for approval, or otherwise. For meetings (other than satellite meetings) scheduled to be held, in the respective region, within one month before or after a meeting of a Regional Associate (American Crystallographic Association, Asian Crystallographic Association, European Crystallographic Association, Latin American Crystallographic Association), the applicants for sponsorship must seek approval of the Chair of the Regional Associate Organizing Committee.

IUCr sponsorship can only be given to meetings that are international in character and open to participants from all countries. For international meetings the membership of the Programme Committee is a good indication of this. National meetings are only supported if held in developing countries.

IUCr sponsorship should only be given to meetings that include a speaker policy and statistics relating to gender balance on the conference website. The policy should be consistent with the IUCr's policy on gender balance and publicize the IUCr Conference Code of Conduct.

Active crystallographers should be involved in the organization of the conference and one or more sessions should deal with specific crystallographic topics. This does not automatically include any session on condensed matter physics, materials science or symmetry not related to crystallography. According to these criteria all meetings organized by IUCr Commissions automatically qualify.

Explicit support from the relevant IUCr Commission(s) is required for any international meeting (except for the meetings of Regional Associates) and from the Commission on Crystallographic Teaching for any international schools (except for those organized by an IUCr Commission).

The IUCr continues to support and uphold ISC's policy of non-discrimination and adheres to its decisions and procedures concerning the free circulation of scientists. Organizers of any meetings seeking IUCr sponsorship or support must assure the Sub-committee on the Union Calendar that the authorities of the country in which the meeting is to take place guarantee free entrance of bona fide scientists from all countries.

Travel support for young scientists is available for all meetings (including schools). This money should not be used for waiver of registration fees or for any purposes other than travel, accommodation and subsistence for the sponsored scientists. For virtual meetings, a lower level of funding will be provided and this can be used to subsidize the cost of online hosting. It is recommended that the presentations of young scientists supported by the IUCr should be in English.

Consideration should be given as to whether the proposed meeting is appropriate in subject, form and timing with respect to other related meetings.

Except in special cases, IUCr funds should not be used to sponsor more than one event per year in the same location.

Registration fees should be the same for both local and nonlocal participants.

*Visiting Professorships.* The IUCr Visiting Professorship Scheme aims to support some of the costs of having internationally recognized scientists as lecturers for short courses at workshops or schools organized in developing countries. These schools or workshops may have national or international character. Up to a maximum of three Visiting Professorships can be granted for a single event. Travel and insurance costs will be met by the IUCr, while the local organizers cover the accommodation/subsistence expenses. Visiting Professorships can be requested in conjunction with the application for IUCr funding of a meeting, or independently as a single action to obtain highly qualified international teaching support within a teaching programme of local character. Support from at least one IUCr Commission is required. Full details may be found at <https://www.iucr.org/iucr/sponsorship/vp.html>.

## 6. Outreach and Education

The IUCr is actively engaged in a number of outreach and education initiatives, targeting several regions worldwide, particularly emerging countries in Africa, Latin America and

SE Asia, and students of all ages, from schoolchildren to early-career researchers and young professors. Such initiatives are held in the spirit of the *Crystallography for the Next Generation* resolution (Morocco, 2015): to build on the success of IYCr2014, the IUCr and partner institutions committed to enhance the stature of crystallography; build capacity in developing regions of the world; and extend further the public understanding of science in general and crystallography in particular.

Some initiatives are described below:

#### *IUCr–UNESCO OpenLabs*

Among the initiatives launched during IYCr2014, the IUCr–UNESCO OpenLabs (<https://www.iucr.org/outreach/openlabs>) proved to be one of the most successful and long-lasting actions. As many as 32 editions have been implemented in 24 different countries so far. In addition to UNESCO, the IUCr has partnered with many companies and institutions on this project. Recent editions since the last IUCr General Assembly held in Hyderabad in 2017 included Senegal, Costa Rica, Côte d'Ivoire, Turkey, Ghana and Benin. All editions planned in 2020 and 2021 were cancelled because of the pandemic. New editions are now on schedule, including the first OpenLab Jordan, to be associated with the SESAME Users meeting.

#### *LAAAMP, Lightsources for Africa, the Americas, Asia, Middle-East and the Pacific*

The IUPAP–IUCr LAAAMP project (<https://laaamp.iucr.org>) was originally funded with a EUR 300 K grant by the International Science Council (ISC). The following tasks have been achieved: (1) preparation and distribution of the brochure 'Advanced Light Sources and Crystallography: Tools of Discovery and Innovation' (versions available: English, French, Spanish, Arabic and Portuguese); (2) over 40 FAST (FAculty-STudent) teams from targeted countries visiting partnering AdLS facilities for a period of two months; (3) participation in strategic science policy meetings (e.g. World Science Forum 2017; CiLAC Forum 2018; World Science Forum 2019) and several other conferences (including the PCCr2/AFLS2 Conference); (4) colloquium presentations given by experts in several targeted countries; and (5) Strategic Plans for the development of AdLS and crystallography in the targeted regions of the project published.

Given the success of the initiatives, the LAAAMP project has been continued and is in full swing. A new partner, the ICTP, has joined IUPAP and IUCr to run the project. The Executive Committee, presently chaired by the IUCr Executive Outreach Officer, has been extended by two new members with the aim of improving its gender and geographical representation. A close collaboration with the African Light Source initiative has been put in place and formalized with an MOU. The SPARC (Synchronizing Partners to Advance Research Characterization) initiative, a mail-in access program to AdLS for researchers from targeted areas of the project, has been launched to overcome problems related to the pandemic. New collaborations have been started, including one with the Canadian Light Source with initiatives directed to high-school science teachers.

#### *X-TechLab, Benin*

X-TechLab is a new X-ray techniques facility established in Benin (<https://www.xtechlab.co/>). It is one of the outcomes of the IUPAP–IUCr project LAAAMP and was initially developed under the framework of the IUCr–UNESCO OpenLab. It was very well received by local authorities, and funded by the government of Benin to be one of the flagship laboratories at Sèmè City (<https://semecity.bj/en/>), the International City of Innovation and Knowledge launched by the Government of Benin in 2016. The initial funding was used to acquire a single-crystal diffractometer, a cryostat and other lab equipment, and to organize some training sessions on crystallography and tomography, which were very successful and attracted participants from the entire Western African region. We plan to organize two such training sessions every year. The last session was held in a hybrid mode, with some students attending in person and lecturers and other participants remotely.

Given the success of the activities and the enthusiasm generated so far, new funding has been made available by the Sèmè City administration for instrumentation. The Scientific Committee, chaired by the IUCr Executive Outreach Officer, has recommended that the X-TechLab acquires a powder diffractometer, which is presently under negotiation.

#### *International Years*

The IUCr is actively participating in the organization of a few festival years to be celebrated in 2022, as follows.

International Year of Basic Sciences for Sustainable Development 2022 (IYBSSD2022). Main organizer: International Union of Pure and Applied Physics (IUPAP). Status: approved by UNESCO in November 2019; expected to be approved by the United Nations General Assembly soon. IUCr involvement: the IUCr Executive Outreach Officer has actively participated in all the preparatory steps, including the organization and co-chairing with the President of IUPAP of a session at the World Science Forum 2019, where the IYBSSD2022 was first announced, and is a member of the Steering Committee. The IUCr is formally a partner of IYBSSD2022.

Year of Mineralogy 2022. Main organizer: International Mineralogical Association (IMA). Status: approved by IMA and seconded by UNESCO, not seeking for approval by the UN. It will be celebrated as part of IYBSSD2022. IUCr involvement: all preparatory steps were conducted by IMA Past President Patrick Cordier and the IUCr Executive Outreach Officer. The IUCr Executive Outreach Officer is presently a member of the Steering Committee. The main event to celebrate the Year of Mineralogy will be the IMA 2022 Conference, Lyon (France), 18–22 July 2022.

International Year of Glass 2022 (IYOG2022). Main organizers: International Commission on Glass (ICG), Community of Glass Associations (CGA), ICOM-Glass. Status: approved by the United Nations General Assembly on 18 May 2021. IUCr participation: the IUCr Executive Outreach Officer and the IUCr Executive Secretary have worked with Professor David Pye (Past President, The American Ceramic Society and Past President, The International Commission on Glass), promoter of IYOG2022, and helped in preparing the ground



for submitting the proposal to UNESCO and the United Nations General Assembly. They are now attending the preparatory meetings to evaluate possible involvement of the IUCr in the programme.

#### *IUCr Newsletter and IUCr website*

As part of the activities of the IUCr Executive Outreach Officer, in collaboration with Brian McMahon, in August 2018 the *IUCr Newsletter* was transformed into a dynamic digital platform with a fresh new look, and the IUCr website (<https://www.iucr.org/>) has been fully redesigned; the new style was launched in 2020. New sections have been added.

**Michele Zema**, IUCr Executive Outreach Officer

## 7. Committee for the Maintenance of the CIF Standard (COMCIFS)

COMCIFS is responsible for maintaining and developing the suite of standards known as the Crystallographic Information Framework (CIF) on behalf of the IUCr. These standards include a data format (CIF), a multitude of discipline-specific dictionaries describing the contents of data files, and the language in which these dictionaries are written (DDLm). The Worldwide Protein Data Bank (wwPDB) is separately responsible for a large and rapidly expanding collection of CIF definitions that encompass concepts and techniques used in the macromolecular community.

At the start of 2021 COMCIFS consisted of five voting members and a broad collection of advisers and observers. The voting members were James Hester (Chair), John Bollinger (Co-Secretary), Brian McMahon (Co-Secretary), John Westbrook, and Herbert Bernstein. A productive COMCIFS business meeting was held online at the end of August following the IUCr Congress. In addition to this meeting, ongoing COMCIFS business was conducted as usual via the associated IUCr mailing lists.

2021 saw the untimely death of long-time voting member John Westbrook. John played a pivotal role in the development of COMCIFS standards over more than two decades, particularly in relation to the wwPDB, whose interests they also represented on COMCIFS. A replacement to represent the macromolecular community is being sought.

#### *Dictionary development*

No new dictionaries were approved this year, and no new data names were added to the core dictionary. A considerable amount of technical development took place, centred around online Github dictionary repositories. Enhancements included automated syntax and semantic checking of dictionary updates. A surprising amount of effort was needed to develop a 'Dictionary Style Guide', specifying precisely how plain-text dictionaries should be formatted: a standard layout makes it simple to assess changes to dictionaries, and to use automated tools for dictionary editing and updating.

The IUCr journals adopted imgCIF as part of a workflow for dealing with raw data files. As part of this effort, extensions to imgCIF were designed for referencing external data, and,

as imgCIF was originally developed as an adjunct to the macromolecular mmCIF dictionary, a way in which imgCIF data names could be combined with data names from the core dictionary was checked and specified.

#### *International Tables for Crystallography, Volume G*

COMCIFS members are closely involved with the preparation of the second edition of *International Tables Volume G (Definition and exchange of crystallographic data)*. This year saw several of the new dictionary chapters move to the review stage, with only one of the new dictionary chapters outstanding. Further information is available in the report of the Commission on *International Tables*.

#### *Interactions with other groups*

COMCIFS is represented on the NeXus International Advisory Committee (NIAC), which primarily develops the NeXus raw data standards for large facilities. No developments relevant to CIF occurred this year. Links were also maintained with the Open Databases Integration for Materials Design (OPTIMADE) initiative, and with the Crystallography domain of the European Materials and Modelling Ontology (EMMO) consortium. As a result of these links J. Hester gave a presentation describing CIF at a related ontology workshop in October.

COMCIFS is also closely involved with the IUCr Committee on Data (CommDat).

#### *Looking forward*

As flagged in previous years, an ever-shrinking group of people is drawn upon to support CIF maintenance and development. This situation is not sustainable, particularly as the first generation of CIF experts move into retirement. Ideas on how this situation might be remedied were discussed with the IUCr Executive Committee and at the August COMCIFS business meeting, and at least some of them should be realized in the near future.

**James Hester**, Chair

## 8. Committee on Data (CommDat)

For 2021 there are the following matters to report:

(i) Various new published reports and announcements have been posted on the IUCr Forum for Public Input to CommDat (<https://forums.iucr.org/viewforum.php?f=39>). These have been extensively accessed.

(ii) CommDat participated fully in the Prague IUCr Congress Programme Committee and organized the two workshops on raw data usage in chemical and in macromolecular crystallography which immediately preceded the Congress. Full details for the events can be found at <https://www.iucr.org/resources/data/commdat/prague-workshop-cx> and <https://www.iucr.org/resources/data/commdat/prague-workshop-mx-raw-data>. The chemical crystallography workshop (August 2021) has led to detailed ideas for next steps, which have been shared with the Chair of the Commission on Structural Chemistry.

(iii) Arising from these two Prague Congress workshops were questions about ownership of unpublished (or unde-

posited) research raw data by a Principal Investigator and/or the measuring experimentalist. It had not been possible to provide answers on this question, so assistance was sought from CODATA at its 2021 General Assembly and this was redirected to the CODATA International Data Policy Committee (IDPC). This in turn led to two detailed discussions with the Rights and Responsibilities subgroup of the CODATA IDPC. The principle at issue was that a Principal Investigator was not necessarily able to delete 'bad' data, such as empty data frames, nor to authorize the timing of release of unpublished raw data. Ownership and control of research data actually varies around the world. The IUCr Journals' *IUCr-Data* new article category Raw Data Letters (Main Editor Loes Kroon-Batenburg, <https://iucrdata.iucr.org/x/index.html>) offers Principal Investigators a new way of publishing raw diffraction data. These articles also offer data reusers a way to collaborate with the measuring team in publishing new analyses of raw data beyond the one initially imagined. A full report of the deliberations with the CODATA IDPC can be found at <https://forums.iucr.org/viewtopic.php?f=39&t=445>.

(iv) The IUCr Executive Committee approved the following new members of the Committee on Data:

Dr Alice Brink, of the Chemistry Department, the University of the Free State, Bloemfontein, South Africa is a researcher in chemical and protein crystallography for targeting new medical imaging agents based on rhenium and technetium; their research encounters data interoperability challenges.

Dr Ian Bruno of the Cambridge Crystallographic Data Centre has strong activity within both IUPAC, the InChI Trust and the Research Data Alliance, with each of which we seek strong synergies and connections which Ian will bring into CommDat.

Professor Genji Kurisu, of the Institute for Protein Research, Osaka University and Director of the Protein Data Bank Japan (PDBj) and its associated raw diffraction data archive XRDa.

Dr Selina Storm, Project Manager of the EMBL Hamburg Beamlines at PETRA IV, an upgraded synchrotron currently being planned which will increase diffraction data rates. Selina is also a developer of high energy diffraction methodology in macromolecular crystallography.

(v) Dr Amy Sarjeant retired from CommDat on taking up a new post in industry. We are pleased to have retained Amy's expertise as a consultant to CommDat and thank them heartily for their contributions to CommDat since 2017.

(vi) The *checkcif for raw diffraction data* initiative has been realized in its core details to accompany the launch of *IUCr-Data*'s new article category Raw Data Letters. This was led by Loes Kroon-Batenburg with the assistance of Andy Gotz at the ESRF (both CommDat members), Fabio Dall'Antonia (EuroXFEL) and James Hester (COMCIFS Chair). We imagine that the availability of this will also assist with synchrotron, X-ray laser and neutron metadata and data archive robustness.

(vii) Close ties remain strong with COMCIFS, the IUCr's technical committee maintaining the CIF standard, which is

chaired by James Hester. James has been a very active member of CommDat and is involved in the Raw Data Letters initiative [see point (vi) above].

**John R. Helliwell**, Chair, and **Brian McMahon**, Secretary

## 9. *IUCr Newsletter*

The *IUCr Newsletter* (<https://www.iucr.org/news/newsletter>) continues to showcase the interests and activities of the IUCr and its Regional Associates and Commissions, and strives to inform, educate and entertain the global community of crystallographers.

This annual report covers four issues: Volume 29 Numbers 1–4 (2021), edited by Mike Glazer. A President's column appeared in all issues, the first two by Sven Lidin and the second two by Hanna Dabkowska.

At the start of 2021 came the news that the 25th IUCr Congress, postponed from 2020, would be held in a hybrid format. In the run-up to the Congress, the *Newsletter* revealed the innovative features that delegates and exhibitors could expect and, post-Congress, published reports and praise for the impressive organization. Other important announcements included the launch of the African Crystallographic Association, and the *Newsletter* also carried reports from the latest two countries to join the IUCr fold, Guatemala and the United Arab Emirates.

Exciting Feature Articles and fascinating historical perspectives accompanied news of IUCr projects, such as the change to the definition of 'crystal' in the *Online Dictionary of Crystallography*. Each issue included articles related to IUCr publications, such as reviews of *International Tables Volume H: Powder diffraction* and the new *Teaching Edition*, information about the transition of *JSR* to full open access in 2022 and the new crystal growth section in *Acta B*.

The number of reports on in-person meetings understandably fell considerably during this period, having hitherto accounted for about a third of the content. However, the average number of items published in each issue in 2021 remained the same as in previous years, and these included several online-meeting reports from organisers keen to share their experiences.

The e-mail editions of the *Newsletter* were circulated to 13 500 crystallographers and structural scientists worldwide, and social-media channels provided additional exposure. The complete *Newsletter* archive is available at <https://www.iucr.org/news/newsletter/archive>.

This period saw the retirement of two Regional Editors: Ted Baker (Asia including Australia, New Zealand and Pacific Island territories) and Serena C. Tarantino (Europe including Russia and the Middle East), whom I would like to thank for their time and help with the relaunch of the *Newsletter* in 2018. Ted has been replaced by Christopher Sumbly, with a view to appointing an additional Regional Editor to represent China, and Serena by Anders Ø. Madsen and Panče Naumov; I look forward to working with them. We also bade a fond farewell to

Patti Potter, who had worked on the publication since it was established in 1993.

Mike Glazer, Editor

## 10. IUCr/Oxford University Press (OUP) Book Series Committee

The Book Series Committee members provided assessments of two new book proposals, one a monograph and one a teaching text, which were then brought together as Chair's reports. These two reports were first provided to the IUCr Executive Committee, which endorsed them, and then they were submitted to OUP. Details are below.

An evaluation was made of a proposal for a research monograph entitled *Crystal Chemistry of High Pressure Nitrides*, by Natalia Dubrovinskaya, Leonid Dubrovinsky (both at University of Bayreuth, Germany), Maxim Bykov (Carnegie Institution, Washington DC), and Dominique Laniel (University of Bayreuth).

An evaluation was made of a proposal for a second edition of the book by Professor Dr Ulrich Müller, entitled *Symmetry Relationships between Crystal Structures*, published in 2013 (in paperback 2017). It is in our IUCr OUP Book Series Crystallography Texts. The OUP website for the book is <https://global.oup.com/academic/product/symmetry-relationships-between-crystal-structures-9780199669950>.

In order to ensure consistency to IUCr nomenclature policies, and to reduce the chance of errors, we have reaffirmed to OUP the need for us to assign volunteer(s) with requisite subject expertise, ideally from our Committee, so as to review a full draft of a new text in our Book Series before publication by OUP in our, *i.e.* the IUCr's, name.

John R. Helliwell, Chair

## 11. Gender Equity and Diversity Committee (GEDC)

At the Prague 2021 IUCr Congress, the General Assembly formally approved the Gender Equity and Diversity Statement that the GEDC drafted. We also farewelled two original members of the GEDC – Dr Ruchi Anand from India and Dr Claire Murray from the UK. We are grateful for their leadership on gender equity and diversity and thank them for the time and energy they put into this committee. The GEDC then welcomed two new members of the committee, Dr Radha Chauhan from India and Professor Catherine Drennan from the USA, and appointed a Deputy Chair, Dr Helen Maynard-Casely (Australia) (the Chair remains with Professor Jennifer Martin, Australia). Dr Maynard-Casely is also a member of the Local Organizing Committee for the Melbourne 2023 IUCr Congress, which is an important consideration.

The IUCr signed up to membership of the Standing Committee for Gender Equality in Science (SCGES) (<https://gender-equality-in-science.org/scges-partners/>). The IUCr Executive Committee has appointed the Chair of the IUCr's GEDC as an *ex officio* IUCr representative of SCGES and

the Deputy representative is Professor Sven Lidin (IUCr Immediate Past President, and a member of the GEDC).

Dr Maynard-Casely and Professor Martin met several times in 2021, to develop and plan for GEDC meetings. The new GEDC has met several times (virtually) in 2021 after the Prague Congress to discuss our priorities and SMART goals (specific, measurable, achievable, relevant, time-limited) for 2022–2023. These priorities will be finalized in early 2022.

J. L. Martin, Chair

## 12. The IUCr Crystallography in Africa Initiative

Owing to the pandemic it was impossible to organize any OpenLabs in 2021. However, we provided equipment to Dschang University, prepared for the ePCCr3 meeting to be held in Kenya in 2023, launched the African Crystallographic Association (AfCA), and promoted remote experiments in collaboration with UNESCO.

### Equipment

#### Dschang, Cameroon

Dr Claude Caucheteux, a Bruker engineer, installed two diffractometers in Dschang that were totally renewed by Bruker. These two diffractometers were given by Bruker and the IUCr's Crystallography in Africa Initiative negotiated free installation. Dschang University contributed with the purchase of one X-ray tube and a computer. The first experiments have been made on a test crystal and were very positive, and Dr Patrice Kenfack and Professor Ignas Tonle from Dschang are now equipping the X-ray lab with microscopes *etc.*, and seeking money to buy electricity power stabilizers; the IUCr and UNESCO might help in 2022.

#### Lomé, Togo

Lomé University will be equipped with a Rigaku powder diffractometer (mostly paid for by the World Bank). Rigaku also installed for free a Nova single-crystal diffractometer given to the community by IPBS, a French CNRS biocrystallography lab, through Dr Valerie Guillet. Dr Ayi Djifa Hounsi (Lomé University) will be in charge of both diffractometers. They should be installed in 2022 and it is planned that the IUCr will pay for the transportation. Dr Hounsi attended three OpenLabs or workshops organized by the Chair of the Crystallography in Africa Initiative, and will spend six months in Nancy, France, in 2022 to complete their crystallography education.

#### Nouakchott, Mauritania

The Mauritanian government is keen to finance and develop research, and to provide funding to equip laboratories. An NMR machine was bought in 2021 and diffractometers will be bought in 2022; therefore a remote lab will be organized. Professor Aliou Hamady Barry will be in charge of this equipment and will also be a lecturer at an OpenLab in Ziguinchor, and is spending three months in Nancy, France, to learn how to use the diffractometers. The remote lab will use a remote connection from Nancy to Nouakchott (see below).

## *Pan African Conference on Crystallography (ePCCr)*

This joint conference between AfCA, the African Light Source (AfLS) and the African Physical Society was held as a virtual meeting in November 2021, see <https://events.saip.org.za/event/170>.

The African Crystallographic Association (AfCA) was launched at the ePCCr, thanks to the efforts of Professor Delia Haynes (Stellenbosch University) and Dr Patrice Kenfack (Dschang University) and their team. This association was first discussed at PCCr1.

## *Promoting remote experiments in collaboration with UNESCO*

A first test for a remote laboratory began in 2021 with Dr Kenfack at Dschang University. Remote experiments link via the internet a laboratory equipped with up-to-date diffractometers anywhere in the world to any African University (or in the future any emerging country). The remote crystallographer will then be able to pilot their own single-crystal or powder diffraction experiment. As they will have gained the necessary expertise before at an OpenLab, they will then be able to collect and reduce the data, solve and refine structures, analyze powder diffraction spectra and publish their own research without a co-author from another institution. They will also be able to teach masterclasses using a PC and a video projection focused on the remote experiment. Therefore remote labs will enable solid-state research in Africa and 'hands-on' experience in X-ray crystallography.

Claude Lecomte, Chair

## 13. Regional Associates

### 13.1. American Crystallographic Association (ACA)

The American Crystallographic Association, Inc. (the ACA) is a nonprofit, scientific organization of 1500 members. It was founded in 1949. The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. For more details please visit the regularly updated, informative and easy to navigate ACA web page (<http://www.amerocrystalassn.org>).

The 2021 ACA Council consisted of David Rose (President), Diana Tomchick (Vice-President), Brian Toby (Past-President), Ilia Guzei (Treasurer), Kushol Gupta (Secretary), and Chelsy Chesterman as the Young Scientists Special Interest Group (YSSIG) representative to the Council (*ex officio*). Gerald Audette served as the Canadian National Committee for Crystallography (CNCC) representative and Thomas Proffen as the IUCr representative (*ex officio*). Kristin Stevens continues as the Executive Director and Kristina Vitale continues as the Membership Secretary. Membership of all committees and officers of all special interest groups are listed in the Spring 2021 edition of *Reflexions* (<https://www.amerocrystalassn.org/reflections-archive>).

In 2021 the Council continued its once-a-month teleconferences because of continuing COVID-19 restrictions. The monthly teleconferences continued to be very successful.

The 71st Annual Meeting of the American Crystallographic Association was again moved from an in-person format to a virtual format (vACA2021). Following the Star Trek-inspired theme from 2020, a Star Wars-inspired meeting theme, 'Structural Science Awakens', was chosen in 2021 to highlight the ACA's new tagline ACA: The Structural Science Society. Nozomi Ando, Carla Slebodnick, Brandon Mercado and Anna Gardberg co-chaired this meeting. The scientific program was held from 30 July to 5 August, with associated workshops 9–16 August. With the remarkable work of many volunteers and organizers, the vACA2021 was able to offer a full scientific program in 2021, with 35 scientific sessions, 4 interactive poster sessions, 5 workshops, speed mentoring for the young scientist, and opportunities for exhibitors to interact with our members during poster sessions and/or corporate webinars. The meeting was well attended with over 600 registrants and over 300 workshop participants. Other meeting statistics are available at <https://www.amerocrystalassn.org/past-meetings>.

The 2021 ACA Award Winners (presented at the 2022 Annual Meeting) were Arthur Schultz (Bau Award), David Goodsell (Fankuchen Award), Airlie McCoy (Trueblood Award) and Brent Nannenga (Etter Award). The 2021 ACA Fellow titles were bestowed on Leighton Coates, Jan Ilavsky, Liang Tong, Lynne Howell, Frank Hawthorne, Richard Gillilan, and Hanna Dabkowska.

The ACA adopted 'The Structural Science Society' as a tagline and a committee was formed to create a new logo replacing the original one created by Helen Berman over thirty-five years ago. The new logo was unveiled in December 2021 celebrating the breadth of science the ACA represents. The logo can be viewed in the ACA home page (<http://www.amerocrystalassn.org>).

The 2022 (72nd) ACA:SSS Meeting will be held in Portland, Oregon, 30 July – 2 August, offering a virtual option.

The ACA/AIP journal *Structural Dynamics* achieved an impact factor of 3.368 in 2021.

The ACA:SSS supported many progressive statements and actions regarding the situation of science and social activities in the USA (often acting together with the APS).

The Canadian National Committee for Crystallography (CNCC) (<http://xtallography.ca/>) is chaired by Tomislav Friscic, the Vice Chair is Louise Dawe, the Secretary is Michel Fodje and the Treasurer is Brian Patrick.

Th. Proffen, IUCr Representative

### 13.2. Asian Crystallographic Association (AsCA)

AsCA continues to play a leading role in the nurturing of collective crystallographic activities in the Asia-Pacific region with successful scientific meetings being held in those years in which there is no IUCr Congress and General Assembly, albeit activities in 2021 were still impacted by the COVID-19 pandemic.



*AsCA Executive Officers*

The Executive Officers for the term 2020–2022 were elected in Singapore (2019) and are Xiao-Dong Su (President, China), Genji Kurisu (Vice-President, Japan), Siegbert Schmid (Secretary/Treasurer, Australia) and Jennifer Martin (Immediate Past President, Australia).

*AsCA scientific meetings in the period 2021 and beyond*

The next AsCA conference is to be held in Korea (Republic of) in October/November 2022 (<https://asca2022.org/>) on Jeju Island (also subject to favourable global development regarding the pandemic as well as travel funds). The AsCA Executive Committee (EC) is in close contact with the local organisers and preparations are going well. Registration will be open on 1 May 2022. Discussions on a hybrid format have been held. Remote presentation and attendance will be available, but the registration fee for online attendance is not fixed yet. If the participants change their minds from on-site to remote presentation, the local organisers will reduce the registration fees and reimburse the difference.

At the Council meeting held in Hanoi (6 December 2016) a proposal was received from the Malaysian representative to host the 17th AsCA Conference at Sunway University, Petaling Jaya, Malaysia, during December 2021. Unfortunately, this conference had to be postponed to 2024, due the COVID-19 imposed travel restrictions.

No conference is planned for 2023, due to the IUCr Congress in Melbourne.

*AsCA Regional Committee Membership*

As Singapore and Bangladesh are in the process of becoming/have become full members of the IUCr, it is planned to include Cambodia and Sri Lanka in their place as members of the AsCA Regional Committee of IUCr (along with Malaysia, Thailand and Vietnam).

An application was received from the crystallographic community in the United Arab Emirates in 2020 for membership of AsCA. This was favourably considered by the EC and approved at the AsCA Council business meeting just before the start of the IUCr's 2021 Congress. The meeting was held on Zoom and had the largest representation across all member countries of AsCA in the history of these meetings.

*AsCA Prize for exemplary contributions to AsCA*

At its 2018 meeting, the AsCA Council approved a proposal by Genji Kurisu (GK) from Japan to offer a prize to honour those who have made an outstanding contribution to AsCA over a prolonged period of time. An AsCA Prize for mid-career researchers was also discussed in the AsCA Council meeting in 2020. These proposals are now being developed in more detail by GK to present to Councillors in the near future.

**Siegbert Schmid**, Secretary/Treasurer

**13.3. European Crystallographic Association (ECA)**

The ECA Executive Committee (ExComm) has collaborated to organize the next European Crystallographic Meeting (ECM33), which will be held in Versailles (23–27 August 2022) with participation in person. Attention has been devoted to including a gender equity topic in the ECM33 scientific

program. The topic will be covered by the Keynote Lecture given by Elspeth Garman (University of Oxford).

The ECA has organized a series of virtual lunchtime webinars taking place every month ([https://ecanews.org/education/eca-lunch-webinars\\_past-events/](https://ecanews.org/education/eca-lunch-webinars_past-events/)).

In addition, the ECA has organized a celebration session dedicated to 25 years of the ECA and 50 years of the European Crystallographic Committee (ECC). The session will take place during the ECM33 Conference on 26 August. It will be carried out as a round-table discussion with all ECA Past Presidents as speakers and P. Beurskens talking about the ECC. The first half of the session will be focused on ECA history, followed by a presentation addressed to future perspectives and crystallography in Europe.

New ECA individual representatives were elected: Philipp Hans (Marseille, France), Kamil Dziubek (Florence, Italy) and Fernando Lahoz (Zaragoza, Spain).

ECA ExComm representatives joined the official constitution of the African Crystallographic Association (AfCA) on 17 November 2021. The ECA President, Professor Marijana Daković, reflected on the strengthening of the African crystallographic community under the umbrella of the ECA and wished them luck and success for future work. Professor Delia Haynes, ECA ExComm member, was elected the first AfCA President.

The European Neutron Scattering Association (ENSA) and the ECA will award two Bertaut prizes in 2022. ENSA and the ECA usually organize the Bertaut award sessions in a regular alternating sequence at ENSA or ECA Congresses, but, due to the pandemic, this could not be realized. The next ENSA Bertaut award has been labelled '2021' and the ceremony will take place during the International Conference on Neutron Scattering in Buenos Aires, Argentina (21–25 August 2022), while the next ECA Bertaut award has been labelled '2022' with a ceremony taking place at ECM33. Max Perutz and Kalman prizes will also be awarded at ECM33.

Due to COVID-19-caused circumstances, the ECA ExComm winter meeting was held online, in February 2022, with discussions on ECM33 Congress organization, ECM34 Congress organizational developments, organization of the 7th European Crystallographic School ECS7 (Lisbon), ECS8 (Berlin) organizational developments, ECA supported events and the ECA's statement on Ukraine.

The ECA ExComm spring meeting has been planned for 29 April – 2 May 2022 in Zagreb, to be held with participation in person.

ECS7 will take place in Lisbon, Portugal, 10–15 July 2022, see <https://ecs7.events.chemistry.pt/>.

The ECA's Statement on Ukraine was published on the ECA website.

**A. Altomare**, IUCr Representative

**13.4. Latin American Crystallographic Association (LACA)**

The country members of the Latin American Crystallographic Association carried out a series of activities during

2021 in spite of the continuing restrictions due to the SARS-CoV-2 outbreak.

LACA had a strong participation in the XXV Congress and General Assembly which took place in hybrid format in 2021. Diego Lamas (Argentina), Abel Moreno-Cárcamo (Mexico), and José Miguel Delgado (Venezuela) did an excellent job representing the region on the International Program Committee. Marcia Fantini and Glaucius Oliva, both from Universidade de São Paulo, Brazil, were Keynote lecturers. They presented, respectively, the lectures ‘The contribution of crystallography to new vaccine formulations’ and ‘A crystallographic snapshot of SARS-CoV-2 main protease maturation process and the discovery of inhibitors’. In addition, crystallographers from LACA participated as microsymbiosia Chairs and Co-chairs and as speakers in different sessions. During the General Assembly, Asociación Cristalográfica de Guatemala (ACriGua) was accepted as a new IUCr member country. It is also worth mentioning that almost all IUCr Commissions incorporated a representative from the LACA region either as member or as a consultant. L. Suescun (Uruguay) was designated as Chair of the Commission on Mathematical and Theoretical Crystallography.

The Argentinian Association of Crystallography (AACr) launched the Eighth Edition of the Crystal Growing Competition on 7 May 2021. Online workshops for participants and elementary and high-school teachers were conducted during May and June. The competition also took place online in 2021 but the 2022 contest will be in person. Eleven teams received awards in four categories and seven honourable mentions in a virtual event on 16 November 2021. The XVI Annual Meeting, XII School (Protein Structure Determination) and IX Workshop (Synchrotron Radiation) of the AACr were also virtual events, streamed from the city of Santa Fe. They were all well attended and very high quality events.

The Brazilian Crystallographic Association (ABCr) celebrated its 50th anniversary with the XXV edition of its meeting (an online event) on 18–22 October 2021. The opening session celebrated past presidents of ABCr. In the following days the program included Plenary and invited speakers from Denmark, France, Italy, Netherlands, the UK, Switzerland, Germany, and Brazil. A short course on Polymorphism in Pharmaceutical Solids and a round-table discussion on the future of crystallography and available state-of-the-art tools were also organized.

The Crystallographic Association of Guatemala organized two webinars: ‘Powder X-ray diffraction. An indispensable tool for the characterization of natural and synthetic solids’ presented by Leopoldo Suescun (Uruguay) on 7 April 2021, and ‘Fundamentals of optical and electron microscopy’ by Shirley Torres and José A. Barillas (Guatemala) on 12 May 2021.

During the months of April, May, and June, the Crystallography Laboratories of Universidad de Los Andes (Mérida, Venezuela) and Universidad Industrial de Santander (Bucaramanga, Colombia) held weekly meetings to discuss basic and advanced features of crystallographic databases, in particular the PDF-4 database and the CSD. These meetings have helped

to strengthen the collaboration between these two laboratories.

It is also important to note that researchers from Ecuador and Bolivia who use diffraction techniques have expressed an intention to form a crystallography society or association. Information about the requirements and procedures have been made available to them and it is hoped that they will soon join the IUCr.

As mentioned before, Union Costarricense de Cristalografía (UCCr) will organize the 2022 LACA meeting and Red Uruguay de Cristalografía (RUCr) will organize the 2024 meeting.

Graciela Díaz de Delgado, IUCr Representative

## 14. Representatives on Other Bodies and Scientific Associates

### 14.1. ICTNS (the Interdivisional Committee on Terminology, Nomenclature and Symbols, a committee of IUPAC)

The Chair of the CCN is a member of the ICTNS.

There did not seem to be any activities of the ICTNS during 2021.

Requests to referee papers and reports submitted to the IUPAC arrive regularly because all submissions are sent to all members of the ICTNS. Most submissions are in specialized areas unrelated to crystallography but a review was written for a manuscript titled ‘Standard Atomic Weights of the Elements 2019’.

Carolyn P. Brock, IUCr Representative

### 14.2. International Science Council (ISC)

The International Science Council has matured quickly since its formation in 2018 from the merger of the International Council for Science (ICSU) and the International Social Science Council (ISSC) in 2018. The IUCr was initially somewhat hesitant in its support of the merger, fearing a weakened role of the natural sciences in this very large organization. I’m happy to write that so far these fears were unfounded and instead, the formation of the ISC was very timely as it was fully operational by the time we were hit by the pandemic and the ISC could assume the important role of speaking for science as a whole. The ISC is certainly emerging as an organization that is well set to work on science for policy and policy for science.

During 2021, the ISC has published an impressive stream of topical reports on current issues: *Resilient Food Systems, Strengthening Science Systems, Enhancing Governance for Sustainability and Rethinking Energy Solutions* in January, *Opening the record of science: making scholarly publishing work for science in the digital era* in February, *Three ways of understanding social transformations to sustainability* in March, *Finding common ground in transformative sustainability narratives* in May, *Unleashing Science: Delivering Missions for Sustainability and Gender Equality in Science: Inclusion and Participation of Women in Global Science*

*Organizations* in September, *Public perceptions and understandings of science, Hazard Information Profiles: Suppl. to UNDRR-ISC Hazard Definition & Classification Review – Technical Report* and *Science as a Global Public Good* in October, *Strengthening research integrity: The role and responsibilities of publishing* in November and *A contemporary perspective on the free and responsible practice of science in the 21st century* in December, as well as a number of reports on the organization itself and its development and goals. The activities of the first three years of operations are recaptured in the triennial report *ISC Activity and Achievement Report: July 2018 to June 2021* from December.

There were no physical meetings of the full Council during 2021, but the General Assembly was held virtually in October and Peter Gluckman, a New Zealand paediatrician was elected President. It is of particular interest to the IUCr that during the General Assembly, Sekazi Mtingwa was awarded the Policy-for-Science Award for their work as *co-founder of a number of important institutions and pan-African programmes, including the African Light Source Initiative*.

The ISC continues to be a grand unifying force for science in society.

S. Lidin, IUCr Representative

#### 14.3. International Science Council Committee on Data for Science and Technology (CODATA)

CODATA is the interdisciplinary Committee on Data for Science and Technology of the International Science Council. Full details of CODATA's activities are available from its website at <http://www.codata.org>. Owing to the COVID-19 pandemic, meetings of CODATA in 2021 were held virtually. Many of the activities of the year for CODATA were recorded and are available on their video channel: <https://vimeo.com/user91439529/videos>. The 2021 General Assembly written reports and the presented slides are at <https://codata.org/events/general-assembly/general-assembly-2021/>. A new feature was the forum of the CODATA national, *i.e.* country, members. The success of that has led to a suggestion for a forum of the scientific unions, which the IUCr would naturally be pleased to take part in. The next International Data Week (IDW) 'Data to Improve our World' is to be held as a hybrid (virtual and in-person) event in Seoul, Korea; it was rescheduled from November 2021 to 20–23 June 2022 (<https://internationaldataweek.org/>). The IDW for 2023 is to be in Salzburg, 23–26th October 2023, entitled 'A Festival of Data'.

Within the CODATA Global Open Science Cloud initiative a case study was proposed involving the Protein Data Bank Japan (PDBj)'s raw diffraction data archive (XRDa). This case study, one of five, was endorsed by the IUCr and approved by CODATA; details can be found at <https://codata.org/initiatives/decadal-programme2/global-open-science-cloud/case-studies/diffraction-data/>.

The efforts to improve the digital representation of units (DRUM) have continued within the CODATA DRUM Task Group (<https://codata.org/initiatives/task-groups/drum/>)

units-of-measurement-for-humans-and-machines/) to facilitate more consistent machine-to-machine usage of units of measurement; human-to-human usage being deemed to be in a satisfactory state. As IUCr Representative to CODATA I have liaised closely with the Chair of the IUCr Nomenclature Committee, Emeritus Professor Carol Brock, who represented the IUCr at the DRUM consultation events, following standard practice that nomenclature and units are considered together.

I was invited by the Executive Secretary of CODATA, Simon Hodson, to present a 5-minute summary on *Provenance in Crystallography* at the Research Data Alliance's virtual Plenary 17 held in April 2021 in a Birds of a Feather Discussion on *Provenance in different science domains*. There were equivalent presentations to my one from other research area domain scientists including chemistry, earth sciences, life sciences, environmental sciences, astronomy and the social sciences. RDA17 had the overarching theme 'Opening data for global challenges'. My slides are at [https://zenodo.org/record/4707690#.YIA-Sj\\_TXIV](https://zenodo.org/record/4707690#.YIA-Sj_TXIV). I am grateful to Brian McMahon at the IUCr's Chester office for discussions preparing for the talk. Brian was the IUCr's CODATA Representative from 2002 to 2012, and retired from the role of IUCr Research and Development Officer in 2021 after 35 years with the IUCr. Brian had a distinguished career at the IUCr and we wish them all the very best in their retirement.

*Digital Representation of Measure (DRUM) Initiative of the Committee on Data (CODATA) of the International Science Council (ISC)*

(The ISC is the successor organization to ICSU. The ISC was formed in July 2018 by the merger of the International Council for Science (ICSU) and the International Social Science Council.)

In July 2020 the Chair of the CCN was appointed to be the IUCr's Ambassador to the DRUM Initiative of CODATA. The official IUCr delegate to CODATA itself is John Helliwell.

A DRUM survey was filled out in May 2021 in consultation with the Chester office and John Helliwell.

John R. Helliwell, IUCr Representative to CODATA, and Carolyn P. Brock, IUCr Ambassador to the DRUM initiative of CODATA

#### 14.4. ISC Committee on Space Research (COSPAR)

COSPAR's (<https://cosparhq.cnes.fr/>) main objective is to promote international collaboration in scientific research in space, with an emphasis on the exchange of results, information and opinions. This organization is responsible for developing world standards for the space environment and its protection.

COSPAR's highest body is the Council. The Council comprises the Committee's President, Representatives of Member National Scientific Institutions and International Scientific Unions, the Chairs of COSPAR Scientific Commissions, and the Chair of the Finance Committee. The Council

meets at the Committee's biennial Scientific Assembly. Between Assemblies on a day-to-day basis COSPAR is run by the Bureau.

COSPAR President for the period 2014–2022 is Lennard A. Fisk (USA) and the Vice President is Karl-Heinz Glassmeier (Germany). Members of the Bureau are: Catherine Césarsky (France), Masaki Fujimoto (Japan), Manuel Grande (UK), Charles Kennel (USA), Pietro Ubertini (Italy) and Chi Wang (China).

The most recent 43rd COSPAR Assembly was held in virtual mode, 28 January 2021 – 4 February 2021 (the original dates and place were 15–22 August 2020 in Sydney). See <https://cospar2021.org/>.

The 44th COSPAR Assembly will be in Athens, Greece, on the 16–24 July 2022. (<https://www.cosparathens2022.org/>.)

The 45rd COSPAR Assembly will take place in Busan, Korea, in 2024.

Following the success of the Capacity Building Workshop (CBW) on Crystallography for Space Science in April 2016 in Puebla, Mexico (<http://www.inaoep.mx>), a similar workshop/school has been proposed for Addis Ababa, Ethiopia, in 2022 or later. Eyasu Leta is the CBW organizer and Yuki Kimura (IUCr) and Carlos Gabriel (COSPAR) will co-chair it.

The Chair of the Scientific Commission on Materials Science in Space (Scientific Commission G) is M. Avila (Germany), and the Vice-Chairs are K. Brinkert, (UK), J. Porter (Spain) and T. Yano, (Japan).

The official journal of COSPAR is *Advances in Space Research (ASR)*, <https://www.journals.elsevier.com/advances-in-space-research>, which had an impact factor of 2.152 in 2020. *ASR* includes COSPAR's information bulletin *Space Research Today*. Another COSPAR journal, *Life Sciences in Space Research*, <https://www.journals.elsevier.com/life-sciences-in-space-research>, had an impact factor of 2.082 in 2020, and is a quarterly peer-reviewed scientific journal covering astrobiology, origins of life, habitability, life in extreme environments, effects of spaceflight on the human body, radiation risks and other aspects of life sciences relevant in space research.

In 2021 COSPAR postponed two CBWs:

Data Analysis for Planetary Sciences, 20–31 July 2020, Antofagasta, Chile.

Pan-Ocean-Remote-Sensing-Conference Tutorial, 15–19 September 2020, Johor Bahru, Malaysia.

The Panel on Capacity Building (PCB) Fellowship program is open to young scientists who participated at one of the COSPAR CBWs, enabling them to build on skills gained at the workshop. It provides for visits of 2–6 weeks duration for the purpose of discussing ideas for a future workshop or carrying out joint research with one of the previously agreed lecturers/advisors of the corresponding workshop.

COSPAR co-organizes a limited number of meetings and colloquia each year that are of interest to its Associates. More information about these initiatives can be found at <https://cosparhq.cnes.fr/events/co-sponsored-meetings>.

**Yuki Kimura**, IUCr Representative

## 14.5. International Standards Organization (ISO)

The Chair of the CCN is a member of the ISO. The group sends out e-mails once a week that list 25–50 reports on a very wide variety of topics (*e.g.*, information technology, plastics and rubber, ships and marine technology, tobacco products, medicinal herbs).

A topic of interest to crystallographers in these reports is very rare, but in early November 2021 the report 'Quantities and units – Part 12: Condensed matter physics' specifically mentioned non-standard usages (ångströms and a factor of  $2\pi$ ) that are widespread in the crystallographic community. Correspondence with Professor Göran Grimvall, the Project Leader, followed. The IUCr was assured that there is no intention to interfere with its current practice. (The version of the report sent out in January 2022 for voting includes the following statement:

It is inevitable that some readers working in particular specialized fields may find that the quantities they are interested in using may not be listed in this International Standard or in another International Standard. However, provided that they can relate their quantities to more familiar examples that are listed, this will not prevent them from defining units for their quantities.

It seems that the ångström is safe.)

A Liaison Report form was filled out in May 2021 in consultation with the Chester office.

**Carolyn P. Brock**, IUCr Representative

## 14.6. International Organization for Crystal Growth (IOCG)

The activities of the IOCG had to be postponed due to the pandemic.

The Executive Committee of the IOCG decided, in view of the pandemic, to move to a date when the 20th International Conference on Crystal Growth and Epitaxy takes place in 2023, from 30 July to 4 August.

**Geetha Balakrishnan**, IUCr Representative

## 14.7. International Centre for Diffraction Data (ICDD)

The Commission on Powder Diffraction maintains close links with the ICDD, and has initiated discussions about how this relationship can possibly be developed into something more substantive and of mutual benefit.

**Dave Billing**, IUCr Representative

## 14.8. Worldwide Protein Data Bank (wwPDB)

The Protein Data Bank (PDB) has been a key resource for macromolecular crystallographers for 50 years, and its policies and development have been strongly influenced by the crystallographic community. Now known as the Worldwide PDB (wwPDB), it comprises five core entities, the RCSB-PDB in the USA, PDBe in Europe, PDBj in Japan, the BMRB (NMR database) and the Electron Microscopy Database (EMDB). The centres collaborate closely and share the load on



deposition, maintaining a single open-access archive that is freely accessible to researchers, educators and students throughout the world.

The wwPDB was formally designated a Scientific Associate of the IUCr in 2015, and the IUCr provides a representative to the wwPDB Advisory Committee (wwPDB-AC). The wwPDB-AC also has representatives from the NMR and cryo-EM communities, as well as regional representation. The wwPDB-AC was chaired by Dr Peter Rosenthal (UK) in 2021.

Professor Ted Baker (New Zealand) was the IUCr Representative on the wwPDB-AC until 2020. In 2021, Professor Jennifer Martin (Australia) (IUCr Executive Committee member) was appointed as the IUCr Representative. The wwPDB Principal Investigators invited Professor Martin to chair the wwPDB-AC from 2022.

The 2021 meeting of the wwPDB-AC was held virtually in October, and some of the major points were:

The archive reached >185 000 macromolecular structures in 2021. The structures continue to grow in size and complexity. About 90% of structures have been determined by crystallography, though the number determined by cryo-EM is increasing rapidly (2952 by cryo-EM in 2021, 9264 by crystallography in 2021). The number of NMR structures remains relatively low in comparison (360 in 2021).

The wwPDB is considering expanding to include PDBc, China, and PDBi, India. Formal decisions on these are expected in 2022.

The PDB celebrated its 50th anniversary (PDB50) in 2021, with celebrations at several events across the globe.

EMBL-EBI (the host of PDBe) and DeepMind co-developed the AlphaFold Protein Structure Database (<https://alphafold.ebi.ac.uk>), a joint project to openly and freely share millions of AlphaFold protein structure predictions (<https://deepmind.com/blog/article/AlphaFold-Using-AI-for-scientific-discovery>) with the scientific community. The database launched officially on 22 July 2021. The initial release contained approximately 365 000 structures, which increased to ~1 million 3D models during 2021. AlphaFold was trained on data from the PDB and other public resources, such as UniProt and MGnify. DeepMind made the AlphaFold structure predictions, source code and methodology freely and openly available to the global scientific community.

**J. L. Martin**, IUCr Representative

## 15. Finances

The Report and Financial Statements for 2021 are given as supporting information.

Transactions denominated in foreign currencies are translated into US dollars (USD) at the rates applying at the dates of the transactions. Monetary assets and liabilities denominated in foreign currencies at the balance-sheet date are retranslated at the rates applying at that date.

Investments are stated at market value. Changes in market value are taken through the income and expenditure account.

The balance sheet shows that the assets of the Union have increased during the year, from USD 4 697 664 to USD 4 861 378. The movement in market value of the investments was a gain of USD 162 783 in 2021 (compared with a gain of USD 79 807 in 2020).

The administrative expenses were USD 228 695 in 2021, as compared with USD 223 224 in 2020.

The only costs for the, largely virtual, Finance and Executive Committee meetings held in 2021 were for travel expenditure for the two members of the Executive Committee who were able to travel to Prague. The subscriptions from Adhering Bodies were USD 194 232. Interest on bank accounts and investments was USD 21 735.

In 2021, the journals showed a surplus of USD 607 898 after journal-development costs were taken into account, as compared with a surplus of USD 1 118 381 as calculated on a similar basis for 2020. The reduction was largely due to an increase in commission taken by the IUCr's publishing partner, Wiley.

The cost of the technical-editing office has been divided between the journals and *International Tables for Crystallography* in percentages based on the staff time spent on each publication. The technical-editing costs for the journals were USD 1 247 469, as compared with USD 1 150 451 in 2020.

Books showed a surplus of USD 46 960, as compared with a surplus of USD 13 850 in 2020. The net sales income for books was USD 155 661 in 2020, as compared with USD 112 360 in 2020.

The cost for the Union in producing the *IUCr Newsletter* in 2021 was USD 7421, compared with USD 8022 in 2020.

USD 10 763 was provided for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union. This was much lower than in pre-pandemic years due to many meetings being postponed or cancelled, with most that went ahead being virtual. The cost of Visiting Professorships (USD 337) was low for the same reason. Outreach and education costs (USD 147 367), which include the value of waivers and discounts for IUCr Journals, contributed to the IUCr's good works in 2021.

An Outreach and Education Fund was established as part of the IYCr2014 legacy. In 2021 donations totalling USD 20 834 were received.