Christopher Sumby

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President's Report



Chris Sumby, SCANZ President

The constitution changes that were discussed as part of the Business Meeting at Crystal35 in Freemantle are to be voted upon in the next month or so. While the Rules that were discussed and voted upon are now in effect, SCANZ members need to formally vote on the changes to the Articles in a full ballot of members. Our hardworking secretary David Turner has been testing a commercial online voting system to ensure that it is fit for purpose (anonymous, secure) ahead of the formal vote. All members will receive an email with instructions and a link to vote. Council have also been working on communications in the first six months of 2025. The first and most obvious change is the format in which you are receiving this newsletter. Michelle Miller, the newsletter editor, will be trialling MailChimp for future newsletters. We believe this will improve the readability and functionality of the newsletter. As we recognise that the pdf newsletters have provided an excellent record of the society's activities, we will ensure that the MailChimp newsletters are suitably archived. Another change that you might have noticed is that we are also on LinkedIn. We'll be increasingly using LinkedIn to share news, make members aware of opportunities (there will still be some emails) and to communicate on matters of interest to the society. Please join the group, which is also open to non-members. Hopefully LinkedIn activity drives a few more researchers and their teams to take up SCANZ membership. If you know of researchers who are not members feel free to forward the newsletter with its encouragement to join (see the end of the newsletter for information). Finally, given we now have an additional communication platform, alongside X(Twitter) and the website, we are looking for a communications officer to help manage the website, LinkedIn and X. If you are interested, please contact me to discuss.

Next year is the Twenty-Seventh Congress and General Assembly of the International Union of Crystallography in Calgary, Canada from the 11th – 18th August, 2026. SCANZ will also run its own meeting in 2026 as part of the shift to a biennial calendar. Crystal36 will take place in Adelaide in quarter four of 2026 (date to be confirmed) and we are investigating holding this jointly with the Australian X-ray Analytical Association (AXAA). I hope to be able to provide more details later this year.

Meanwhile, key affiliated conference dates include:

- AsCA 2025 in Taipei, Taiwan from the 1st 5th December, 2025.
- 27th IUCr in Calgary, Canada from the 11th 18th August, 2026.
- Combined Crystal36/AXAA Meeting, Q4, 2026

SCANZ is on LinkedIn!



SCANZ is now on LinkedIn!

Check out and join our new group on LinkedIn.

Science Meets Parliament



Read about it on <u>LinkedIn</u> and check out some more photos. by Stephen Moggach

Science Meets Parliament (SMP) 2025 in Canberra was an incredibly rewarding experience, made even more significant as I attended on behalf of SCANZ. As a recent Australian citizen, this event provided a unique and insightful window into the intersection of science and policy within our federal government.

The SMP app proved to be an indispensable tool, streamlining the entire event with detailed meeting schedules and delegate profiles. The provided resources, including the "runway sessions" on effectively pitching complex scientific concepts, and the expert advice on preparing for parliamentary meetings, were invaluable. I particularly appreciated the communication strategies shared by Dr. Lila Landowski and Tanya Ha, which were directly applicable to conveying the importance of crystallography.

A significant highlight was my meeting with the staff of Senator Glenn Sterle, Senator for Western Australia. This provided a firsthand understanding of how scientific input, particularly from fields like crystallography, can influence policy decisions. Preparing for this meeting, utilising the comprehensive delegate handbook, was essential for effectively communicating the priorities of structural scientists in Australia, where we spoke for some time on the support for the physical sciences.

Witnessing the Senate in action offered a real-world perspective on parliamentary processes. The gala dinner was also a wonderful opportunity to network with fellow scientists and policymakers, and the atmosphere was truly celebratory. Hearing from Vice Chancellor of Canberra University, Bill Shorten, was also a very memorable experience, as he gave a very honest opinion on the role that scientists must play in developing policy. With areas such as Artificial Intelligence, PFAS pollutants, and nuclear energy at the forefront of minister's minds.

The event fostered a strong sense of community and collaboration, and connecting with delegates from diverse scientific backgrounds was incredibly enriching. I particularly appreciated the opportunity to learn from the experience of ATSE CEO Kylie Walker and NSTC member Associate Professor Jeremy Brownlie, as they shared their expertise on parliamentary engagement.

Attending SMP 2025 on behalf of SCANZ allowed me to advocate for the crucial role of crystallography in advancing scientific discovery and technological innovation. The combination of structured meetings, informative sessions, and networking opportunities made this a truly valuable experience. I left Canberra with a deeper appreciation for the intersection of science and policy, and a renewed enthusiasm for representing SCANZ and contributing to Australia's

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scientific future. I would really encourage the members of SCANZ, if given the opportunity to attend this meeting. Without the financial support of SCANZ I would not have been able to attend, and for that I am very grateful.

I'd like to thank Science & Technology Australia for organising such an impactful event, and I look forward to the next opportunity to engage with the scientific and political communities.



Vale Stephen Harrop

Stephanie Bird, Eleanor Campbell, Thomas Caradoc-Davies, Daniel Eriksson, Yogesh Khandokar, Santosh Panjikar, Alan Riboldi-Tunnicliffe, Chris Szeto, Rachel M. Williamson, Rosemary Young.

Dr Stephen Harrop, who passed away on November 17th, 2024, was a highly respected macromolecular crystallographer whose distinguished career spanned three notable periods. His scientific journey began when he undertook a B.Sc. in Physics at the University of York, before continuing his education by undertaking his PhD at the University of Manchester's Department of Chemistry. He moved half-way around the world to Australia to undertake a Postdoctoral position at the University of New South Wales, before concluding his career as a beamline scientist at the Australian Synchrotron.

Stephen graduated with first-class honours degree in physics and joined the group of John Helliwell as a PhD student in the field of protein crystallography at the University of York. In January 1989, he moved to the University of Manchester's Department of Chemistry, as John had been appointed Professor of Structural Chemistry in a joint role with the UK Synchrotron Radiation Source (SRS) at Daresbury Laboratory. Stephen proved to be an exceptional PhD student. The work presented in his thesis made several important contributions to synchrotron Laue methods for protein crystallography, notably how he explored MAD phasing strategies, and included key work on the structure of concanavalin A and hydroxymethylbilane synthase.

In 1995, Stephen moved to Australia and began his postdoctoral career at the University of New South Wales in Sydney. Stephen joined a brand-new team tasked with building a protein crystallography laboratory. Over his first two years, Stephen played a pivotal role in developing the laboratory and solved the first four structures from this group: the serpin PAI2 in both its stressed and relaxed states, the cryptophyte light harvesting protein PE545, and CLIC1. Stephen was known for his meticulous approach to crystallography, acquiring and processing diffraction data at high resolutions, often around 1.0 Å.

Stephen was an excellent mentor, during his time at the University of New South Wales and later at the Australian Synchrotron he trained numerous undergraduate and doctoral students as well as fellow postdocs and collaborators, where he encouraged them to solve structures independently through his patient guidance. Many of his students have gone on to successful careers in structural biology.

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Stephen found an ideal environment for his way of working when he joined the MX team at the Australian Synchrotron, where his skills were put to full use. He brought together his deep understanding of crystallography with his self-taught programming expertise, which contributed to both the evolution of new capabilities at the synchrotron and subsequent development of software for the MX beamlines. Stephen played a central role on the Macromolecular Crystallography beamlines, where he supported researchers from across Australia and Asia. His contributions to the software that powered the beamlines greatly improved efficiency, enabling groundbreaking discoveries in the study of proteins and biomolecules.

Stephen's rigorous problem-solving skills were matched by his genuine interest in helping others. Whether assisting with code debugging, advising on experimental design, or sharing programming techniques, he was always ready to offer support. His belief in empowering others, coupled with his ability to communicate complex concepts in simple terms, made him an exceptional mentor to both colleagues and users of the synchrotron.

Stephen was known for his kindness, generosity, and dry sense of humour. With a sharp wit typical of his Northern roots, he knew just how and when to lift spirits with his well-timed one liners.

His humility, coupled with his deep passion for science, earned him the respect and admiration of those around him. He had a unique ability to make people feel valued, from seasoned scientists to newcomers, and his mentorship and friendship has left a lasting impact on all of those who met him. Stephen leaves behind a legacy of scientific excellence, collaboration, and mentorship.

He is survived by friends and colleagues, as well as the many crystallographers whose careers he influenced, and the broader community whose work he enriched. His presence will be deeply missed by all who had the privilege of knowing him.

A memorial service for Stephen was held by his colleagues and family at the Australian Synchrotron on Tuesday, November 26th 2024.

Science Communications Committee

Rosemary Young Who are we?

In the lead up to the IUCr2023 congress the Bragg Your Pattern Project was formed, with the aim to share our love for crystallography to primary aged children. This project ran a nation-wide pattern competition and promoted the sharing of every-day patterns through the hashtag #BraggYourPattern, before building up to a pop-up crystallography festival during the congress in Melbourne. Maybe you remember the Big Diamond?

After the congress was over, we wanted to continue what we started and build on the lasting legacy of the congress to continue to support ongoing outreach efforts by the crystallographic community. At the SCANZ General Meeting at Crystal35, the Sci-Comm committee was officially established with the purpose to communicate the science of crystallography and its outcomes to audiences in Australia and New Zealand beyond the academic sphere.

The current committee members are Helen Maynard-Casely, Bronte Johnstone, Rosemary Young and Stuart Batten.

What do we do?

The goals of the SCANZ Sci-Comm committee are to find opportunities to talk about crystallography and its impacts to the public, maintain an outreach website with resources for both the public and crystallographers wishing to conduct outreach, and oversee the organisation of an outreach event at each Crystals meeting. This last item was actioned immediately after the Crystal35 meeting in Fremantle, with Bronte and Rosie visiting 2 local primary schools, Attadale Primary and Nedlands Primary.

Three activities were run for each group of students, firstly an introduction to crystallography and what a crystal scientist does, then building diamond models with kits made from the disassembled Big Diamond, and finally making cubic, body-centered cubic and hexagonal lattices out of lollies and toothpicks.

At Attadale Primary school the activities were run with a Year 4 (32 students) then a Year 3 (36 students) class. The Year 3 students were challenged by building the diamond structure and could relate the shape of the crystal models made to the 3D shapes they had been learning. The Year 4 students had been learning about rocks in science, and so had some understanding of crystalline minerals. They were very excited to learn about all the different types of things that can be crystals too!



The visit to Nedlands Primary School ran slightly differently, starting off with a presentation to all the year 4 and 5 students in the school – over 100 kids! There were lots of questions about crystals, including some tricky ones! After this, we separated to go into two year 5 classrooms to run the diamond and lolly activities. The older students were extended by joining their individual diamond models together (and avoiding making Lonsdaleite).

We went through 6 kg of lollies and ~2000 toothpicks, and a good time was had by all!

Thank you so much for today! The kids have not stopped coming up to me and talking about the session they had with you!

I was wondering if you wouldn't mind sending me the PowerPoint you used from today. I am going to do a shortened version of your lessons today if that's ok? I feel bad for the other year 4 class, as they've all been hounding me!! **Tanaya Barnes, Science Specialist, Attadale Primary School**

What's next?

From the start, structure model kits from the Big Diamond project were intended to be distributed across primary schools in Australia and New Zealand. While (for the most part) the Big Diamond is disassembled and kits are ready to be sent out, we want the kits to be accompanied by detailed, useful and user-friendly booklets so that the kids and teachers can get the most out of their model kits. To this end, we have been working with a graphic designer to produce these and get them professionally printed. We are aiming to finish this process and send out kits to schools by the end of this year.

	Contents	
Where did all the 'atoms and bonds' come from?		
In 2023, the work's crystallographers came to Motionare for a large international conference, hosting by the Society for Charal Socialization and New Zaaland (SCANZ). As part of this event we launched the Bings Your Pattern papers (two Marging Your and Income) lange and the social social social social social (principally people under 11) rars of (b) the exerce of crystallography and (c) and (c) a	Welcome 3 Benuer Kin Graphite 8 Making your own crystal functions models structure Graphite Graphite	$\bigcirc \frown \bigcirc \frown$
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Peotro Cessori Jun Alshima	Every time you write you leave about 1.000 layers of graphite behind (depending on how hard you push	
During the conference, scientists from all over the world and school kids from around Melbourne helped to build it. When finished, the model had:	your pencit).	$ \rightarrow $
62,356 121,547 24 341kg	How to use this kit	\smile \smile
Atoms Bonds Layers In weight	This booklet has self-guided instructions for students to build five different structures with the kit, and instructions for more are hosted on our website.	The layers are made up of tiny pieces that are all the same.
The model was disastembled after the conference and then packaged up to these kits to send to schools in Australia and New Zealand. All the atoms and bonds in this set were part of a world record!	The first status (Binchare 1 – Guaha) is very much a whole class satisfy, that could be understand inscribe tab, are probably best understates as walf groups.	They are something called carbon. Have you haved of carbon before? Where else do you think it might be found?

If any SCANZ members are interested in running their own outreach activities, the Sci-Comm committee can assist with activity plans, teacher resources, diamond model kits, and experience running these activities for a range of ages and group sizes. We are also planning on storing a "Crystal-a-Con" in a box kit in each state/region in Australia and New Zealand, so that members across our geographical range have access to the physical resources, as well as the online ones, needed to run their own crystallography outreach activities. Please get in contact if you are interested in this program.

AsCA2024 Maslen Awardees

Ben Krinkel

Attending the AsCA 2024 conference in Kuala Lumpur was undoubtedly one of the highlights of my year. Presenting my research to an international audience was an incredible experience, and I thoroughly enjoyed immersing myself in the local culture and cuisine. The drug discovery and disease-related protein structures sessions were particularly memorable, with standout talks from Peter Czabotar on BCL-2 and Kurt Krause on the remarkable 20,000-fold activation of a bacterial cell wall protein. Additionally, networking with colleagues from Australia and across the Asia Pacific

region was invaluable, leading to the formation of lifelong connections. I am deeply grateful for the funding that made this enriching opportunity possible.



Aston Summers

As my first conference overseas, ASCA 2024 was a fantastic experience with a range of sights, interesting talks and great people. I was a little apprehensive travelling by myself, but after arriving everyone I met was very friendly and the area around the convention centre was interesting to explore. I really enjoyed delivering my talk on lowtemperature high-pressure x-ray diffraction, particularly in a session full of diverse and interesting talks. There was a such a wide range of talks throughout ASCA that really displayed the abundance of everything that is possible with crystallography. Petra Bombicz's talk stood out to me on 'What is Isostructurality?'; a seemingly straight forward technical term that led to quite a thought-provoking talk. The conference dinner was an incredible experience, taking place at the top of the Kuala Lumpur tower with an amazing view over the city.

On a different note, exploring the Kuala Lumpur food and nightlife with the other Australians and New Zealanders was a really enjoyable way to spend the evenings with the Jalan Alor food street being an absolute highlight. I am really grateful to SCANZ for the opportunity to be able to travel to ASCA 2024 and for fostering such a fantastic and inclusive community.



Zannati Zaoti

I attended the AsCA 2024 conference held in Malaysia, where I had the valuable opportunity to present both an oral presentation and a poster. This was my first time attending an international crystallography conference abroad, and it was an incredibly enriching and memorable experience. The conference brought together researchers from across the Asia–Pacific region and beyond, offering a dynamic platform to learn about cutting-edge developments in structural biology and crystallography. Presenting my research in both formats allowed me to receive constructive feedback and engage in meaningful discussions with experts and peers. Traveling internationally for such conferences can be financially challenging, and I am grateful for the support of the Maslen award, which helped make my participation more accessible and the journey smoother. This opportunity not only broadened my scientific knowledge but also strengthened my professional network and confidence in communicating my research.





Katherine Davies

In December 2024, the SCANZ Maslen award supported my attendance of the 18th conference of the Asian Crystallographic Association, in Kuala Lumpur, Malaysia. Some structural biology highlights were Kurt Krause's talk on a novel pseudomonas therapeutic. It had beautiful structures and very interesting biochemical data. I also enjoyed Sun-Shin Cha's keynote talk, featuring a novel protein fold that he crystallised from a thermophilic Archaea – I love that there are still new folds to find!

I felt very nervous about delivering my presentation on the Wednesday, but afterwards I was happy with how it went, and grateful for the opportunity.

Our Malaysian hosts put on a wonderful conference for us, with a very thrilling opening ceremony (the gong and smoke machine were next level!), and enjoyable conference dinner. I found the view of the Kuala Lumpur Skyline from the top of the Kuala Lumpur Tower absolutely stunning.



CSD Data and Software Update

<u>The latest CSD update —CSD 6.00</u> brings significant advancements, including a new data format that is extendable, faster to search, contains more data and is smaller to download.

It includes 1,371,757 entries, with 45% organic and 55% metal-organic structures.

Notably, over 165,000 CSD entries now feature fully calculated disorder models, allowing for improved visualization and analysis of disordered structures.

Additionally, existing entries have been enriched with new searchable fields to enhance their scientific value and analytical potential.

This release also includes:

- <u>Covalent docking enhancements in GOLD</u> and ligand overlay in the CSD Python API.
- New powder X-Ray diffraction functionality.
- CLP force field added to VisualHabit in CSD-Particle.
- 4 new CSD Subsets: Generally Recognised as Safe (GRAS) substances, retracted entries, semiconductors and entries with associated raw data DOIs.

Latest Blogs and Videos

Enriching the CSD: New Data Fields for Deeper Structural Insights

The Cambridge Structural Database (CSD) 6.00 features new searchable fields that enhance existing entries, providing greater scientific value. You can now identify relevant structures more easily, with new data integrity fields added for over one million entries from submitted CIFs.

Bringing Order to Disorder: Expanding Structural Detail in the Cambridge Structural Database

We are improving how disorder is represented in the Cambridge Structural Database (CSD). Read on for the enhancements, challenges faced, and the significance of accurately capturing disorder for structural chemistry and data-driven research.

How to: Search Scientific Literature with the CSD

New to the CSD, about to teach students orguide undergraduate research projects? This video introduces the database, itscontents, and how to search and download data to help enrich scientific studiesand inspire new directions of research.

Upcoming Webinar

Frontiers of Chemistry Education Panel Webinar: Preparing Students for Emerging Career Paths

Technology is evolving faster than ever before, and with it, science career paths change too. How can educators, institutions, and students best prepare for career paths that may not yet exist?

Join our panel to explore key questions for chemistry students and educators, to learn how to best prepare for the future of work and careers.

Thursday 4th September 2025

- 2am NZST (New Zealand)
- 12midnight AEST (Melbourne, Sydney, Brisbane)
- 11.30pm ACST (Adelaide)
- 9pm AWST (Perth)

Register Now

Meet the Team - Upcoming Events

- 18–23 July 75th ACA Annual Meeting 2025
- 25–29 August European Crystallographic Meeting 2025 (ECM35)

The Cambridge Structural Database (CSD) is celebrating its 60th anniversary. We are hosting numerous events throughout the year to mark this significant occasion. Meet us at the 75th ACA annual meeting and ECM35 as we invite our community to celebrate with us, reflect on our past, and look toward the future.

Established in 1965, the database includes historical structures dating back to the 1920s. Our global community has been vital to the growth of the database, which now contains over 1.3 million accurate 3D structures, derived from X-ray and neutron diffraction analyses, and additional curation by The CCDC.

Check our events page for more updates throughout the year!

What do you think about our new

newsletter format? Let us know!

Start Survey

New Members Welcome!

SCANZ warmly welcomes new members. Benefits of membership include:

- Global representation through AsCa, IUCr and STA
- Prestigious awards
- Discounted conference fees
- Exceptional generous student travel support
- Information and job vacancy sharing
- Membership from as little as \$10 per year for students.

Membership applications can be made through the <u>SCANZ website</u>. Contact your friendly SCANZ committee members if you require a sponsor for your application.

SCANZ Committee

President: Chris Sumby (christopher.sumby@adelaide.edu.au) Past President: Charlie Bond (charles.bond@uwa.edu.au) Vice-President: Emily Parker (emily.parker@vuw.ac.nz) Secretary: David Turner (david.turner@monash.edu) Treasurer: Jack Clegg (j.clegg@uq.edu.au) Council Members:

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