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Société Suisse de Cristallographie
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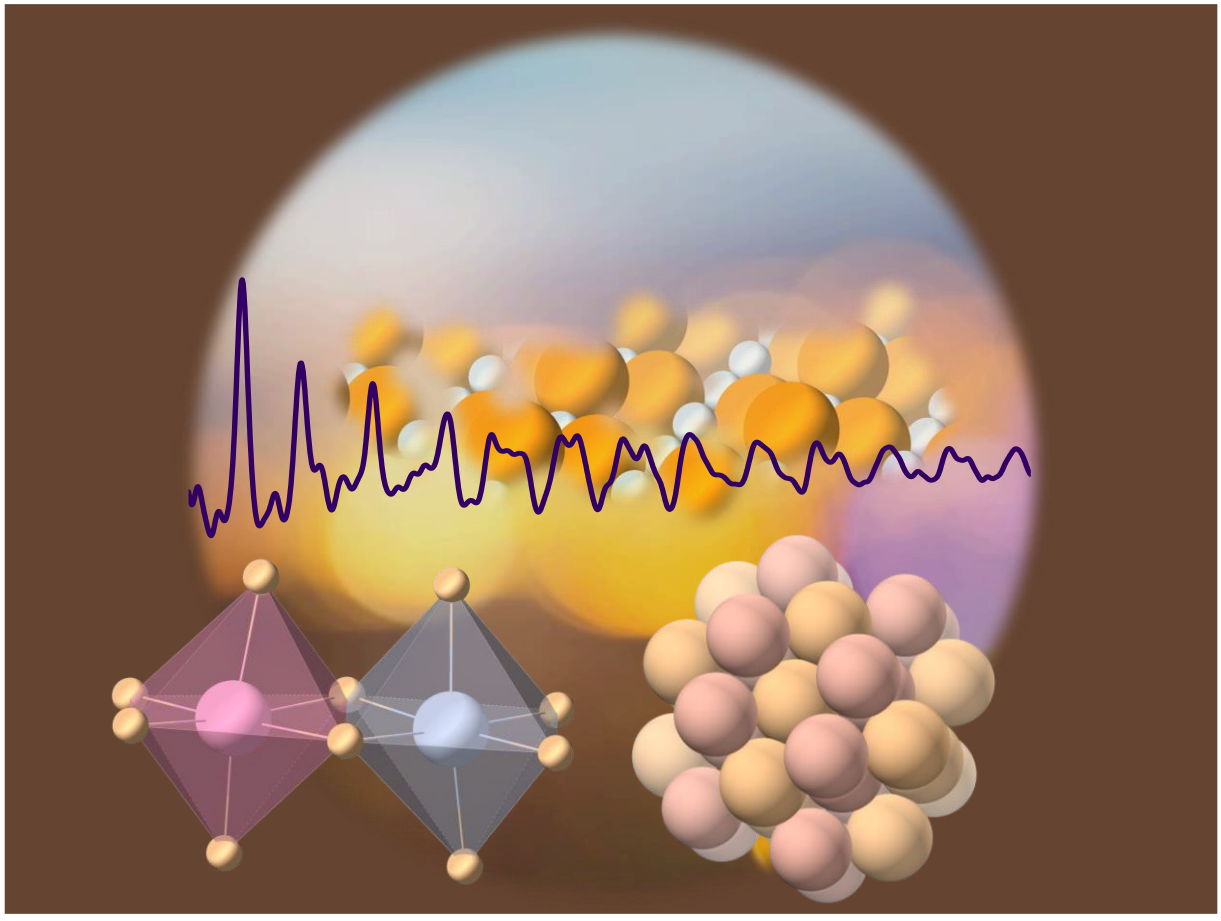

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SSCr workshop in Melbourne IUCr 2023
SAXS workshop at ETHZ, organized by the SSCr
Lecture Series 2023: pair distribution function analysis

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The President's Page

Dear members,

I hope you have all had a good start into the year, enjoying the nice weather and snow, provided you found any. 2023 is going to be a busy and exciting year for the society, and I look forward to the new initiatives, which I summarize for you down below, and their outcome.

Some months ago, I had the pleasure of attending a lecture that ended with the message "crystallography is everywhere". Possibly sounding a little simplistic, maybe regarded as an oversell, this could very well serve as a mantra to the current and next young generation of young crystallographers. X-ray scattering methods and applications using crystallographic tools have indeed found their way into nearly every space of the natural sciences, from arts and archeology to virology and planetary science. The lecturer in question was my Ph.D. supervisor Radovan Cerny, and the talk in question was his farewell lecture at the University of Geneva, end of last year. While I wish Radovan all the best for his retirement, with a ton of good wind and snow on the lake and in the mountains surrounding Geneva, this lecture also marks the end of the last Laboratory of Crystallography in Switzerland awarding a PhD title in the discipline. This is not at all a reason to be nostalgic. On the contrary, Crystallography is everywhere, and the number of researchers using it, knowingly or unknowingly, increases every day. The challenge is creating awareness and redistributing responsibilities in their education, wherever this is no longer ensured by dedicated research chairs and regular University curricula.

As society it is our mission, and in our interest, to use our resources and network in order to help closing educational gaps. Something that was dear to my heart during my presidency was to work on the creation of a workshop satisfying the evolving needs of young colleagues, and responding to them on an annual basis. I'm delighted to notice that our board is on a good way with this. A small building block in a much larger puzzle, yet I am convinced that these are activities our society needs to identify, support and organize, along with our members and corporate partners. With this in mind, last year's panel discussion in Bern explored the needs and opinions of a representative student pool, and the obtained feedback could be summarized into topics on local order, and nanoscopic order. We will launch this workshop prior to our annual meeting at the University of Zürich in September, with Small Angle X-ray Scattering. Still in line with last year's student feedback, the 2024 edition will deal with Total Scattering. The stage will already be set in 2023 by the Howard Flack Crystallographic Lecture Series, which will be given by Simon Billinge from Columbia, NY, beginning of November. I'm very much looking forward to meeting Simon and am

sure his lectures will go well beyond the basics of pair distribution function analysis. Please reserve the date.

Our board has also been busy with setting up a satellite workshop at the 26th Congress of the International Union of Crystallography in Melbourne, which was accepted and is now available for registration on the conference website: “A practical approach to synchrotron experiments”. This is representative of our effort in improving our outreach. The same goes for our social media, where we appear to be one of the most followed crystallographic associations in the world! Swiss Crystallography is literally everywhere!

As usual, I remind both private and corporate members that we want to foster communication, and contributing to our newsletter is one way to do so.

I wish you a good spring and hope to see you soon,

Pascal Schouwink

Pair Distribution Function Analysis in the Laboratory

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The pair distribution function (PDF) analysis of X-ray (neutron or electron) total scattering data is a valuable technique to characterize the local to the mid-range structure of a broad range of materials [1]. This information is essential for a fundamental understanding of many materials' properties as well as for developing novel materials and synthesis routes. In the past decades, PDF analysis has greatly benefited areas such as solid-state physics, energy materials, geology, pharmaceuticals and chemistry, including catalysis.[1, 2] X-ray-based PDF studies have been mostly performed at synchrotron radiation facilities which provide high photon flux of high energies (> 30 keV) allowing excellent counting statistics up to high *Q*, and hence, fast acquisition times (e.g. ranging from seconds to minutes per scan). Even though the number of beamlines dedicated to PDF analysis has grown significantly in recent years, access to these facilities remains limited, restricting the number of materials that can be explored by PDF. On the bright side, with recent advances in laboratory X-ray diffractometers, PDF analysis is available daily for our research. Such instruments are nowadays accessible worldwide, notably in Switzerland at different research institutions. Here, we present a perspective on the use of laboratory-based instruments for PDF analysis.

What information does PDF analysis provide? The PDF gives a real-space insight into the short-to-intermediate-range structural correlations (typically 0.1 - 7 nm) using both the Bragg peaks and the diffuse scattering present in the total scattering data. The PDF describes the probability of finding two atoms separated by a certain distance in the material under investigation. This approach is very valuable to investigate non-crystalline, nanocrystalline or crystalline materials with local symmetry-breaking materials.[3, 4]

What are the experimental requirements for PDF? The basics of PDF are well documented in the literature.[1, 3, 5] Here, we briefly discuss a few key practical experimental considerations. For PDF analysis, we collect total scattering data optimized for a high maximum momentum transfer *Q* ($Q = 4\pi\sin\theta/\lambda$, where θ is half the scattering angle, 2θ, and λ the X-ray wavelength). The PDF (also called G(r)) is obtained by applying a Fourier transform to the total scattering structure function, F(Q), see inset in Figure 1. To obtain F(Q) we collect a diffraction pattern, subtract the incoherent background and apply several corrections to the data as described in detail elsewhere.[5] Typically, the maximum Q measured (Q_{max}) should be above 17 – 20 $Å^{-1}$ to obtain structural information on the atomic scale with sufficient real-space resolution and to minimize truncation errors, which are negligible for $Q_{max} \geq 30$ $Å^{-1}$. The larger the

probed Q-range, the more accurate information can be extracted. Thus, PDF experiments are conducted with hard radiation and up to high scattering angles. Both a high incident photon flux and efficient detectors at these high photon energies are important for obtaining good signal-to-noise at high Q as well as a careful minimization of the (non-sample related) background.

What are the advantages and the limitations of laboratory-based PDF? Modern laboratory-based X-ray diffractometers can reach high enough Q_{max} (e.g., up to 21 $Å^{-1}$, using an Ag X-ray source, or 17 $Å^{-1}$ using a Mo X-ray source) and with recent development of detection systems and optics, high-quality PDF data in laboratories can be obtained.[6, 7] The relatively low costs, availability of laboratory setups and the broad range of possible applications make them a convenient alternative to synchrotron experiments. These instruments are useful as preliminary studies that can strengthen a proposal for synchrotron measurements, as a complementary measurement to previously acquired synchrotron-based data or as a full research study.[8] For certain studies requiring a Q_{max} higher than 21 $Å^{-1}$, a synchrotron will still be required, yet preliminary tests in a laboratory can accelerate sample screening for a more efficient synchrotron beamtime. Furthermore, laboratory setups are important educational instruments, allowing the extension of knowledge not only to PhD students but also to bachelor's and master's students. When compared with synchrotron-based X-rays, lower photon fluxes in in-house equipment leads to a lower signal-to-noise ratio, which must be compensated by long acquisition times. On the other hand, time is not a limiting factor in many cases, i.e. for static measurement under ambient conditions. Moreover, these instruments have been designed for optimal background suppression which is a key benefit for PDF analysis, and they offer a very stable configuration. The latter is not always the case in the beamline facilities configuration as the setup may change from user to user in regular basis (e.g., due to installation of non-ambient setups, accessories, or changes in the X-rays wavelengths). For *in situ* time-resolved studies, synchrotron radiation is key since it provides high photon flux of high energies allowing us to have good counting statistics up to high *Q* and fast acquisition times.[9] However, for systems that do not change significantly over short periods of time (in the time scale of hours), laboratory PDF under non-ambient conditions can bring further opportunities via customized configurations.

Data acquisition. In addition to the vast literature,[3-5] the instruments' manufacturers typically provide excellent guidelines for the good practice of PDF data collection in the laboratory. However, a few general practical considerations can be outlined. Data collection protocols should be optimized for each material system and diffractometer setup in terms of step size and acquisition times. In fact, the total acquisition time can vary considerably from material to material in the order of hours to days. The degrees of crystallinity, the sample density and the scattering factor of the constituent elements impact the signal-to-noise ratio of the data collected. Importantly, the signal-to-noise ratio must be evaluated from the reduced structure function F(Q) at high Q values.

PDF experiments are typically performed in transmission (Debye–Scherrer geometry) in which the sample is mounted inside a thin-walled capillary, (commonly borosilicate glass or Kapton), for which absorption by the sample must be considered when

choosing the capillary size. For air-sensitive materials, the capillaries can be sealed inside a glovebox. In some cases, fluorescence background (for example, when working with Ag radiation, elements such as Pd, Rh, Ru or Mo give a fluorescence background) must be considered and properly suppressed, typically by setting an energy threshold using an energy-discriminating detector. Finally, another aspect to consider is the reciprocal space resolution for the determination of finite nanoparticle size determination. In these studies, instrumental dampening must be first evaluated by measuring a standard (such as LaB_6) under the same setup, limiting the maximum nanoparticle sizes that can be determined and the use of monochromatic Ag $K_{\alpha 1}$ radiation is advantageus.[6]

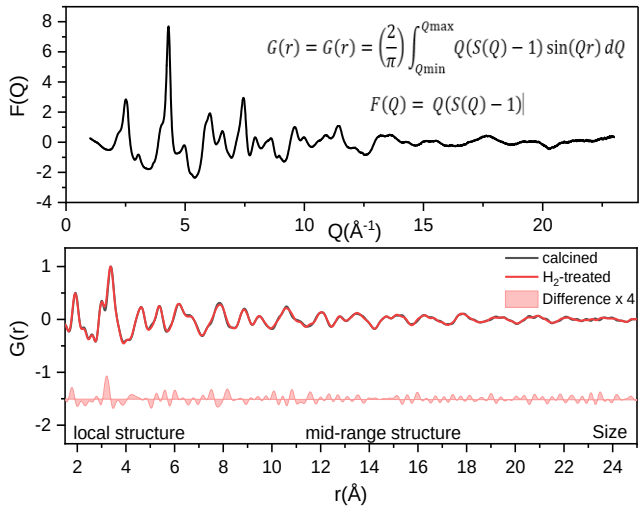

Figure 1. Top. F(Q) of Ga_2O_3 (2.5 nm) nanoparticles after calcination (600°C). The inset shows the equation to obtain G(r) where S(Q) is the total scattering function and F(Q) the reduced scattering function. Bottom. The corresponding G(r) together with the material treated in H_2 (500°C) and the difference G(r) between the calcined and H_2-treated nanoparticles (Data collected using an Ag-based diffractometer Empyrean – Malvern-Panalytical, with a total acquisition time of 22 h). Adapted from [8].

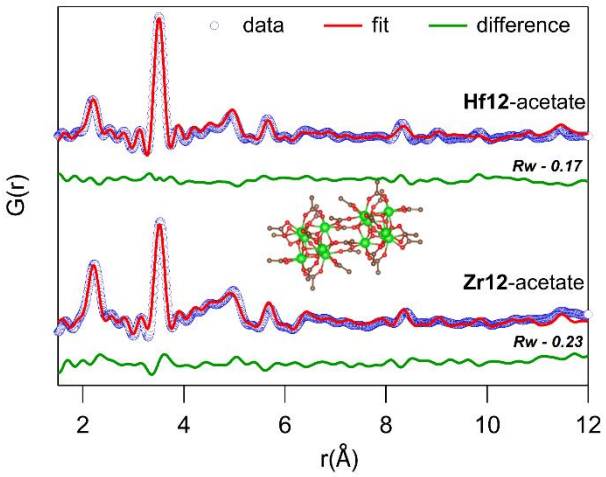

Figure 2. G(r) of $[M_6O_4(OH)_4(OOCMe)_{12}]_2$ (M = Zr or Hf) oxo clusters and their structure. Data collected using an Ag-based diffractometer Empyrean – Malvern-Panalytical, with a total acquisition time of 41 h).

Application examples. In the following, we showcase three recent applications of the use of laboratory-based PDF to the analysis of the material's structure at the nanoscale.

Disorder in Ga_2O_3 nanoparticles. A recent publication evaluated the local structure of γ-Ga_2O_3 (2.5 nm) nanoparticles produced via a colloidal synthesis method by PDF analysis using a laboratory-based system.[8] The goal was to evaluate possible changes in the nanoparticle structure after H_2 treatment (Figure 1). The PDF analysis showed no appreciable changes in the intermediate range structure of the nanoparticles (8 – 20 Å) indicating that the γ-phase was largely preserved after the H_2 treatment, while slight variations in the local range, at ca. 3.1 – 3.5 Å were related to an increased degree of defects (more disordered) related to the formation of oxygen vacancy sites.

Size Determination of metal oxide nanocrystals. When the composition of the nanocrystals consists of reasonably heavy

atoms (with a high scattering cross section), the data quality of the source instruments approaches that of synchrotron data, and can be used directly for publication. For example, the size of ZrO_2 nanocrystals, synthesized with surfactants, was determined by refining the data against a model of a periodic tetragonal crystal structure (P42/nmc) with an envelope function to capture the nanocrystal size.[10] Excellent refinements were obtained with a goodness of fits close to synchrotron data.

Structure determination of metal oxo clusters. Metal oxo clusters are atomically precise collections of metals, held together by oxo bonds. They are used as secondary building unit in MOF, but also exist as discrete structures. Discrete metal oxo clusters share structural features with both inorganic complexes and ligand-capped nanocrystals. While traditional structure determination relies on single crystal diffraction, zirconium and hafnium oxo clusters can also be characterized by PDF, with data acquired via lab sources. The advantage of PDF analysis is its general applicability, even on non-crystalline samples. One can take a discrete model of the oxo cluster and refine its structure against the data, see Figure 2.[11]

Conclusion. Laboratory diffractometers are useful instruments that can provide detailed structural information of complex materials at the nanoscale complementing synchrotron-based studies, accelerating materials development and data analysis, and optimizing the relatively scarce beam time at the synchrotrons.

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Report SGK/SSCr Annual Meeting 2022

The 2022 Annual Meeting of our Society took place at the University of Bern, Department of Chemistry, Biochemistry and Pharmaceutical Sciences, on September 15th. There were about 100 participants and six exhibitors (Rigaku, Bruker, Stoe, Eldico, Dectris and Malvern-Panalytical), so the meeting was fortunately at full capacity again, not impaired by Covid-19 complications. We could also resume the tradition of the conference dinner on the night before with about 40 participants at the restaurant Altes Tramdepot overlooking the beautiful old town of Bern above the river Aare.

The scientific program was a bit different to previous years. There was, for example, a round-table discussion between postdocs and PhD students in our field, moderated by our President Pascal Schouwink (left photo), to find out about the most suited topics for the upcoming SSCr workshops, which will in the future always be held one day before the Annual Meeting. This was very informative, and we could pin down the topics for 2023 (small-angle X-ray scattering) and 2024 (pair distribution function analysis).

There were three sessions with oral contributions: Materials and minerals (invited speaker: Prof. Enrico Mugnaioli, Pisa), structural biology (invited speaker: Prof. Andreas Engel, Basel) and chemical crystallography (invited speaker: Prof. Simon Parsons, Edinburgh, see right photo). In addition, the large user facilities in Switzerland were introduced with short talks by leading scientists.

UNIVERSITÄT BERN

Happy retirement, Radovan!

August 1st, 2022 marks the retirement of our colleague and friend Radovan Černý (University of Geneva). Radovan will continue some of his activities as an Emeritus Professor, but chances are better that you may find him searching for new minerals in the mountains surrounding Geneva, or on his boat, either enjoying the erratic winds of the neighbouring lake, or the apéritif on the boat when there are none. If you are close you might be invited to his chalet, and be allowed to participate in a jam session or be sent into the garden to pick fresh vegetables.

Radovan's career as a crystallographer began during his doctoral studies, which he finished in 1987 at Charles University in Prague (Czech Republic), under the supervision of V. Valvoda, studying alloys of hard materials based on carbides, nitrides and oxides of titanium with X-ray powder diffraction. In 1989-1990, as a young fellow at the Inst. of Mineralogy, University of Göttingen, he then specialized in the study of TiN's thin film microstructure and developed the texture correction in Seemann-Bohlin diffractometry.

He moved to Switzerland shortly after, first as a post-doctoral fellow, then as MER in the Crystallography Laboratory of the University of Geneva (seen during his farewell lecture in the image below), becoming a close-neighbour colleague of Howard D. Flack, famous for his chirality studies by diffraction, and to whom the SSCr dedicates an annual lecture series.

A lifestyle scientist in a way, Radovan's scientific interests have always been broad, going from the crystal chemistry of intermetallic compounds and metal hydrides (a particularly complex intermetallic structure family derived from $YbCu_{4.5}$ bears the name "Černý phases") to the methodological development of powder diffraction applications (the well-known FOX software, developed by V. Favre-Nicolin, was a brainchild of Radovan's), with excursions into modulated structures and total scattering.

In 2012 Radovan became an associate professor and began focussing his group's research on solid-state electrolytes which they synthesized, and characterized crystallographically and thermodynamically. His group discovered excellent candidate solid-state electrolytes for Na-ion batteries, making use of the simplicity of rules governing crystal chemistry. Some of these champion materials, composed of closo-dodecahydridoborate anions, made it into the radio, newspaper, and YouTube in recent years, to the delight of colleagues and friends from a broad circle.

The mineral Radovanite, part of the characterization of new mineral species, is another "crystallographic pleasure". Thanks to Halil Sarp from the *Musée d'histoire naturelle* of Geneva, Radovan got in touch with what he considers "the most beautiful job in the world": the mineralogist, spending half your time in the mountains looking for minerals and the other half solving crystal structures. By determining the crystal structure of nine new minerals Radovan followed a dream, and inspired the name of a beautiful green mineral of the chemical formula unit $Cu_2Fe^{3+}(AsO_4)[As^{3+}O_2(OH)_2]\cdot H_2O$.

Many of us know how invested Radovan has been in the Swiss landscape evolving around crystallography, and phrases like "…why not ask Radovan…" will surely remain part of our community's habits. Radovan has been instrumental in the development of methods and facilities for crystallography, for which we are grateful.

Our farewell message to Radovan:

> *We warmly thank Radovan, for being an active member of the Swiss society for crystallography, on the board committee, as our president (in 2003-2005), and more generally in the worldwide crystallographic community. Radovan wanted to organize EPDIC10 in the Swiss mountains but turned out hosting a wonderful conference in Geneva. We hope to bring EPDIC19 to Switzerland, this time in the mountains and we count on your presence.*
>
> *We trust you will continue sharing the pleasure of crystallographic knowledge with your colleagues and the younger generations, as you have done. We wish you all the best for your very active new retirement life!*
>
> *Keep in touch!*
>
> *All of us*
>
> *SSCr*

2022 Crystallographic Howard Flack Lecture Series

Like many things, the Flack Lectures were able to regain their original format in 2022, meaning on-site lectures with meetings, lunches, dinners and generally a lot of exciting interaction between the Flack Lecturer and colleagues. The pandemic years also saw some exciting technical developments that concern small molecule crystallography, which consists in starting to make structural investigations by electron crystallography available to the broader user-pool, thanks to the commercial availability of user-friendly electron microscopes optimized for such structural studies.

For the Swiss Society for Crystallography, it was thus a cherry on the cake to welcome Lukáš Palatinus (Institute of Physics of the Czech Academy of Prague), who visited Switzerland from 7-11. November 2022. Lukáš, who previously spent some years a long time ago at EPFL in Switzerland, during which he wrote the software Superflip, enjoyed returning for a busy week of well-visited lectures (40-80 participants) at six institutions, starting at ETHZ, PSI, University of Basel, University of Bern, EPFL, University of Geneva.

His lectures focussed on the theory and practice of 3 D electron diffraction, in particular structural refinements using the dynamic diffraction theory, and included absolute structure determination from 3D ED data as well as first results on charge density analysis, thus venturing beyond the current “routine” applications of 3D electron diffraction. These lectures attracted not only routined small molecule crystallographers and macromolecular crystallographers, but also many colleagues working on nano-materials, as well as electron microscopists, seeking information on this tool highly complementary to other microscopic techniques. Both the topic and the audience were thus genuinely pluri-disciplinary, which ensured stimulating discussions, on some occasions well beyond the foreseen time schedule. Lukáš facilitated this by including something for everyone, and discussing the prospects as well as the limits. This was much appreciated by the audience.

The Flack Lectures will stick with crystallographic methods designed to investigate nanomaterials in 2023, their 6th year, for which we are looking forward to welcome Simon Billinge from Columbia, NY, as our 2023 Flack lecturer. Simon will be speaking about total scattering and surely have some interesting insight into using big data tools on the pair distribution function. The program will be communicated soon, please reserve the week of 06.11.2023 (see the announcement on page 19).

Pascal Schouwink

Top: Lukáš Palatinus enjoying the apéro with Dieter Schwarzenbach after his lecture at EPFL. Bottom: First Flack Lecture of 2022, at ETHZ.

SGK/SSCr Travel Grants 2022

We congratulate the recipients of the travel grants in 2022: Yaser Balmohammadi, University of Bern, Justine Schwarte, University of Fribourg and Dr. Aurelio Borzì, Empa. Herby, the awardees share their impressions of the scientific meeting in which they participated and presented their works.

ICDM9 by Yaser Balmohammadi, University of Bern

12-16th of June 2022

Left to right: Professor Dylan Jayatilaka, Dr. Simon Grabowsky, Yaser Balmohammadi

Last year Swiss crystallography awarded me a travel grant and provided me with a great opportunity to participate in an amazing conference in Aarhus city in Denmark, the 9th International charge density meeting (ICDM9). This conference Is the most important scientific gathering in my research field, quantum crystallography. For me was really wonderful to meet a lot of great professors in person whom I only knew their name by reading their papers. For example, professor Dylan Jayatilaka from Australia or Professor Piero Macchi who was at Bern university for a long time. The conference was held for 5 days, and I had a contribution to a poster. During the time of the conference, I listened to fantastic talks, had interesting discussions with others, and got very constructive feedback about my own research. Besides the scientific part, we could enjoy the beauty and sightseeing of Aarhus city together. I would like to thank the Swiss crystallography society for this award which provided the financial base for me to attend the ICDM9 conference.

EuChemS Congress 2022 by Justine Schwarte, University of Fribourg

28th August – 01st September 2022

Justine Schwarte

The organization of the Chemistry Congress 2022 by the European Chemical Society took place in the beautiful city of Lisbon at the end of last Summer. The conference gathered chemists with various domains of expertise, from material chemistry to organic synthesis and including metal-containing compounds or analytical methods.

Different parallel sessions were the opportunity to listen to the last advances of research in central fields of chemistry, when plenary sessions were hold by notorious scientists who highlighted the key points of their work. Without doing an exhaustive list, we can cite

Professor Michele Parrinello who is using crystals of Li_2NH to stabilize the storage and release of dihydrogen. Professor Lutz Ackerman presented the use of a ruthenium catalyzer to generate multiple C–C bonds, meaning the possible recovery of protons and electrons for redox or electrochemical applications. Last but not least, Professor Hanadi Sleiman was interested in the formation of stable DNA cages, her work evolving further in the synthesis of solid fibers or triple DNA helices.

With so many speakers in a few days, the conference program was dense, but we did not miss time to have fruitful discussions with other attendees during breaks and posters sessions.

Finally, I was particularly impressed by the Pátio da Galé where the congress dinner was hold. This reception room, with transparent roof in front of the Tagus was a lovely place, and the dinner was well animated by talented singers.

I am deeply grateful to SGK for having supported my participation to this conference through a travel grant. Get the opportunity to present my work there as an oral communication was a great chance, and I came back with several new ideas to pursue my research.

EPDIC17 Aurelio Borzì, Empa

31st May – 03rd June 2022


Dr. Aurelio Borzì

I am a Postdoctoral researcher at the Center for X-ray Analytics of Empa and I was awarded by the Swiss Society for Crystallography a travel grant to participate in the 17th European Powder Diffraction Conference (EPDIC17), which has taken place from the 31st May – 03r June 2022 in Sîbenik (Croatia). The talk was focused on “Influence of Deposition Methods and Parameters on the Microstructure of Highly Epitaxial Pt Thin Films” which highlighted the relevance that crystallographic methods applied to complex materials systems play in leading the optimization of the microstructure of materials and related devices' performance. The work was presented in the MS “Stress-strain, texture and thin film” chaired by Prof. David Rafaja.

The conference has seen the participation of about 300 delegates from all over the world and represented a superb scientific event not only for the powder diffraction community but in general for researchers active in all the fields of crystallography. Topics of actual interest in the crystallographic context such as total scattering, pair distribution function analysis, structural analysis of proteins and biomolecules,

quantum crystallography, electron and neutron diffraction, and defects analysis in thin films, have been covered during the three full days of extremely interesting talks and poster sessions.

Remarkably, the format of the conference allowed participants to follow most of the contributions, which represented a great opportunity for learning, exchange, and networking.

Lecture Series 2023

Swiss Society for Crystallography

The Howard Flack Crystallographic Lecture Series
On the topic:
Local Structure

The 2023 Howard Flack Lecture Series will focus on local order and pair distribution function analysis with Professor Simon Billinge as our invited Flack Lecturer. As a materials scientist, Simon uses and advances crystallographic techniques to study local-structure property relationships across many different materials used for energy, catalysis, environmental remediation, and pharmaceuticals.

November 6th to November 10th, 2023
Professor Simon Billinge, Columbia University
Talks at five or more Swiss institutions

Schedule and locations soon on:
swiss-crystallography.ch/en/flack_lectures and twitter.com/Swisscrystallog

Simon's research focuses on the study of local-structure property relationships of disordered crystals and nanocrystals using advanced X-ray and neutron diffraction techniques. In particular, he is a leader in the development of the atomic pair distribution function (PDF) method applied to complex materials. These methods are applied to the study of nanoscale structure and its role in the properties of diverse materials of interest, for example, in energy, catalysis, environmental remediation and pharmaceuticals. The approach is to use advanced X-ray, neutron and electron scattering methods, utilizing some of the world's most powerful sources, and applying advanced computation and analysis, including artificial intelligence, machine learning, and graph theoretic methods. A major activity is the study of the nanostructure inverse problem (NIP) where the goal is to obtain the 3D arrangement of atoms from structures with nanoscale atomic structures from scattering data, and the synthesis inverse problem, where the goal is to find an unknown synthesis recipe

given a desired material product. These are non-trivial ill-posed inverse problems that require novel applied math and computational approaches to solve.
Source: https://www.apam.columbia.edu/faculty/simon-billinge

The **Howard Flack Lecturer Award** is conferred annually by the Swiss Society for Crystallography on a scientist who is making or has made significant recent contributions to the field of structural science or involving the use of structural science in the chemical, biological, physical, medicinal or materials sciences. The awardee is then normally invited for a week-long tour of Switzerland to present seminars as part of The **Howard Flack Lecture Series** at several Swiss institutions and research facilities.

The Howard Flack Lecture Series was created by the SGK/SSCr in 2018 in honour of **Howard Flack** (1943–2017), a colleague and a friend, who is remembered for his enormous contributions to crystallography and structural science in general and to Swiss science in particular. This initiative has attracted interest from the Swiss Academy of Sciences (Platform, Mathematics, Astronomy and Physics, to which we belong), which partially sponsors the lecture series.

Howard undertook his PhD studies with Kathleen Lonsdale at University College London, then worked as a research assistant in the Cavendish Laboratory in Cambridge, UK. How better to become interested in research and crystallography? He moved to the Laboratoire de Cristallographie at the University of Geneva, Switzerland in 1971 and spent the rest of his career there. David Watkin and Dieter Schwarzenbach eloquently describe his life and work in *J. Appl. Cryst.* **2017**, *50*, 666.

Howard made many significant contributions to the field of crystallography, but is perhaps best known for his seminal ideas concerning the determination of absolute structure by X-ray diffraction, which originated in 1983, but were constantly being improved upon and extended until his untimely passing. Prior to 1983, it was challenging to determine the absolute configuration of chiral organic molecules, even though this information was vitally important for many chemists and for the pharmaceutical industry, in particular. Howard developed a robust mathematical algorithm, which improved substantially the ease and reliability of the absolute structure determination. This algorithm is now incorporated in all of the usual software and produces a value, now known widely as the Flack parameter, which most people take for granted these days. This development is described articulately by David Watkin in Tetrahedron: *Asymmetry* **2017**, *28*, 1189. Additional information on absolute structure determination can be found in A. Linden, Tetrahedron: *Asymmetry* **2017**, *28*, 1314 and references therein.

Howard was a humble man, who had a special sense of humor. The Swiss Society for Crystallography is proud to name an award and lecture series in his honor.

Announcement of the SGK / SSCr Annual Meeting 2023

7th September: **Workshop** (page 22) and Conference Dinner,
8th September: Conference

Irchel Campus, University of Zurich, Zurich Switzerland
Winterthurerstrasse 190, 8057 Zürich

Format: On-site.
Registration and Invited Speakers will be announced in our web site.

See you soon in Zurich!

Announcement of the SSCr Workshop 2023

Swiss Society for Crystallography
Workshop – 07.09.2023, University of Zürich

Small Angle X-ray Scattering

SSCr workshop on SAXS principles and applications, 07.09.2023

With introductions to:

- SAXS instrumentation, lab and synchrotron based
- Data reduction and basic modelling
- Software tools and approaches
- Applications in inorganic and biological sciences
- Lab visit

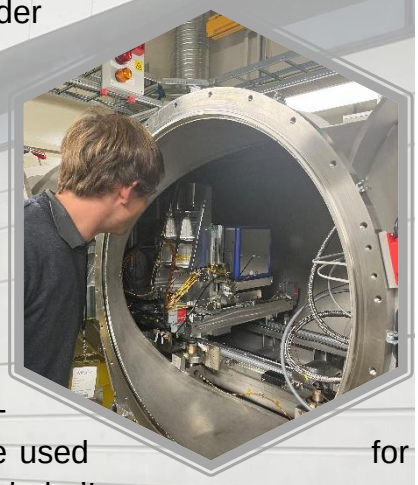
The workshop is intended for graduate and postgraduate students, newbies to the subject, with speakers from academic research labs, synchrotron facilities and companies supplying SAXS equipment. Topics will be discussed in an introductory manner, including examples and/or demos. Participants will be provided with information on where to follow up in detail on different subjects.
The workshop will end with a lab tour at ETHZ (Hönggerberg campus) followed by a dinner. Participants are invited, and encouraged, to join the annual meeting of the Swiss Society for Crystallography the day after, 08.09.2023.
The workshop will be held on-site only.
Registration open soon on: https://swisscrystallog-saxs2023.epfl.ch

Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Swiss Society for Crystallography

Announcement of the SSCr - IUCr workshop "Practical approach to synchrotron experiments"

A half-day workshop will be held in the frame of the IUCr congress on 21.08.2023. Six speakers (scientists and beamline scientists) give practical advice and guidance to synchrotron users in all stages of the beamtime: pre-experiments, experiments, and post-experiments.

The workshop on "Practical approach to synchrotron experiments" aims to answer pragmatic questions that synchrotron users may have when trying to optimize their beamtime. These include finding a suitable beamline, access mode to synchrotrons, proposal writing, designing, and conducting an experiment, troubleshooting during the measurement, and post-experiment activities. As such, the workshop is suited for a range of audiences: first-time users, researchers without immediate contact at synchrotrons, advanced users aiming to improve their use of beamtime, and users from the industry. Six speakers, researchers and beamline scientists, will share their advice and provide guidance in a form of short lectures. There, the audience can learn how to optimize beamtime for various applications: powder X-ray diffraction, SAXS/WAXS, (total) scattering (PDF), macromolecular crystallography and small molecule crystallography. During lunch, there will be time for further discussions with speakers be it specific questions on the technique or what can we learn from other techniques.



The workshop is organised in collaboration between the IUCr committees and the Swiss Society for Crystallography and it will take place on 21.08.23, 8:00-13:00. Melbourne. The registration fee (40 AUD) will be used for lunch and coffee catering during the workshop. Lunch included!

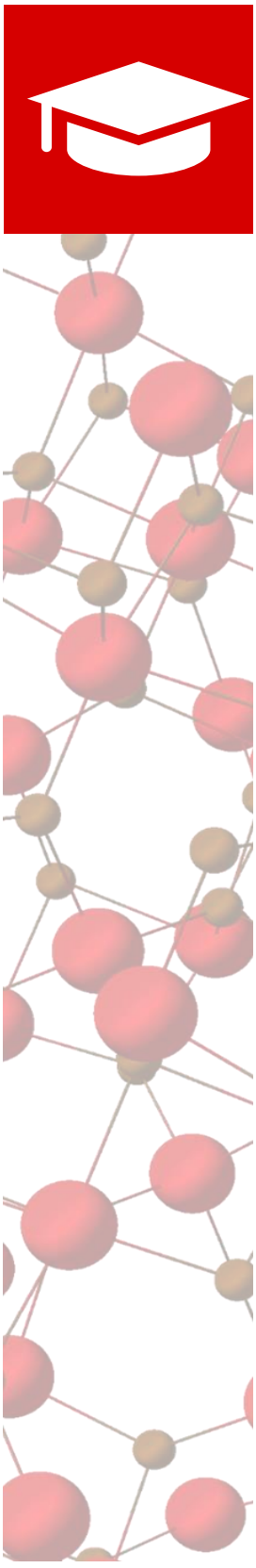
Applications for the workshop can be made using the IUCr portal:

https://iucr2023.org/workshops/

We are looking forward to seeing you in Melbourne!

DECTRIS is acknowledged for the sponsorship.

Announcement of the SSCr PhD prize



The Swiss Society for Crystallography awards outstanding doctoral theses in crystallography

Call 2023

Requirements

The prize is open to:

- Students, of any nationality, who earned a PhD title from a Swiss University
- Students, of any nationality, who earned a PhD title from a university abroad, but carried out a significant amount of work for the PhD title at a Swiss research institution or facility.
- Students of Swiss nationality who earned a PhD title from any University worldwide.

The candidate must have earned the PhD title no earlier than three years before the application deadline and no later than two months prior to the application deadline. The subject of the thesis can be in any area of crystallography and structural sciences (including structural biology, chemical crystallography, solid-state physics, well as the investigation of nanocrystals, metacrystals, quasicrystals, amorphous and 2D materials, etc.). Scientific excellence and implications of the obtained results for crystallography are prerequisites.

Applications

The application for the prize should be submitted before **April 30, 2023**, by the student or by the thesis supervisor. The applicant should submit:

i. a copy of the thesis;
ii. a letter of the supervisor approving his/her candidature;
iii. copies of the articles published from the results obtained during the thesis);
iv. the PhD diploma (or an official certificate of thesis acceptance);
v. a short CV of the candidate (max 2 pages).

All the documents should be submitted in .pdf format via e-mail to the secretary of the SSCr: **swiss.crystallography@gmail.com**.

Award

The winner will be selected by a Jury, based on the excellence of the research, the quality of the publications, and the active contribution of the candidate to the scientific work. The winner will be announced before the annual SSCr meeting and will be invited to give a talk to present the results of his/her thesis. The SSCr will award the winner a diploma and will reimburse the participation of the student in the SSCr annual meeting. The prize includes a financial sum of CHF 2000.

Travel Grants for SGK/SSCr Scientists

Our Society is supporting members participating at international conferences, workshops and schools.

Conditions for travel grants for young SSCr members (under 35):

- Only current members of the SSCr can be supported financially
- Student members can get up to CHF 500 for a poster presentation and CHF 750 for an oral presentation. Attendance at a workshop or school outside Switzerland, if the program does not permit participant presentations, can be supported with CHF 500.
- Postdocs can be supported only for oral presentations with a maximum of CHF 500

Per institute and year, a maximum of two persons can be supported.

Please submit applications to the President of the Society via swiss.crystallography@gmail.com including the following:

- conference abstract if applicable, type of presentation/involvement and letter of motivation
- letter of support from your supervisor
- brief budget of expected costs of attending the meeting
- specify the date you first joined the SSCr

A 1-2 page scientific report for the SSCr newsletter is expected within 2 months of the meeting.

Financial support can also be granted to retired SSCr members:

- Active participation at an event is required: e.g. presentation, lecture, session chair, organizer
- Young researchers have priority if our budget is limited
- The grant amount will be decided by the board, depending on the available budget

Meetings, Conferences, Workshops, Schools, Courses

SAXS Excites Symposium 2023 and Non-Ambient XRD Workshop

4 - 5 Apr 2023

Graz, Austria

www.anton-paar.com/ch-fr/saxs-excites/

Hot Topics in Contemporary Crystallography 5: Experimental advances in macromolecular crystallography

16 - 21 Apr 2023

Dubrovnik, Croatia,

https://htcc5.org/

First Masuku Remote Crystallography Openlab

16 – 23 May 2023

Gabon, France

http://univ-masuku.org/openlab/communication.pdf

8th European Crystallography School

18 - 24 Jun 2023

Berlin, Germany,

https://ecs8.ecanews.org

The ***18th International Summer School on Crystal Growth*** will be organised in **Parma**, the Italian Capital of Culture 2020-21, as an in-person event, after the change of date imposed by the pandemic emergency.
The **Campus of Science and Technology of Parma University** has been chosen to host this event. A friendly and stimulating environment will facilitate discussions and new contacts between lecturers and participants.

As per tradition, the School is organized in conjunction with the **International Conference on Crystal Growth and Epitaxy**, which takes place in Naples in the following week.

Registration is now open!

School's **Program** will be constantly updated in the next weeks.

https://isscg-18.unipr.it

info-isscg-18@unipr.it

18th International Summer School on Crystal Growth

23 - 29 July 2023

Parma, Italy

isscg-18.unipr.it

International Conference on Crystal Growth and Epitaxy

30 July - 4 Aug 2023

Naples, Italy

www.iccge20.org/

26th Congress & General Assembly of the International Union of Crystallography 2023

22 - 29 Aug 2023

Melbourne, Australia

www.iucr2023.org

The 34th European Crystallographic Meeting, ECM34

26 - 31 Aug 2024

Padova, Italy

www.ecanews.org/

SSCr-SGK Annual Meeting and Workshop

7 - 8 Sep 2023

Zurich, Switzerland,

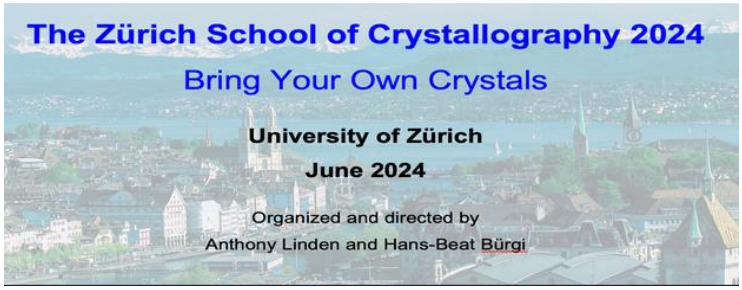
www.swiss-crystallography.ch

2023 Synchrotron Powder Diffraction School at PSI

11 - 15 Sept 2023

Villigen, Switzerland,

www.epfl.ch/research/domains/ccmx/courses-and-events/2023pds/



Jun 2024

Zurich, Switzerland,

Applications for the Zurich School of crystallography June 2024 will open in October 2023 www.chem.uzh.ch/linden/zsc/

The 34th European Crystallographic Meeting, ECM34

26 - 31 Aug 2024

Padova, Italy

www.ecanews.org/

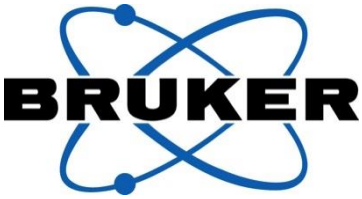
Calls for proposals at large scale facilities

Beside normal proposals, most facilities allow urgent beam time requests. Please check directly with the facility. (tba = to be announced)

Facility	Deadline(s)	Link
SLS		
All except non PX	suspended	
Protein crystallography (PX)	suspended	
SINQ/SLS	suspended	
Joint x+n proposals (MS/HRPT)		
SINQ		https://www.psi.ch/de/useroffice/proposal-deadlines
All instruments regular calls	15.05, 15.11	
SμS: Swiss Muon Source		
DOLLY, GPD, GPS, HAL-9500, LEM	01.06, 01.09	
SwissFEL		
ARAMIS-Alvra, ARAMIS-Bernina	15.03, 15.09	
ESRF		
Standard proposals	01.03, 10.09	http://www.esrf.fr/UsersAndScience/
Long Term Project and HUB proposals	16.01	
CRG SNBL	01.03, 10.09	www.esrf.fr/UsersAndScience/Experiments/CRG/BM01# For more details on the access mode to SNBL: wouter@esrf.fr
ILL	tba	www.ill.eu/users
FRM II All instruments/ Rapid access program	tba	http://www.mlz-garching.de/user-office/
SNS Oak Ridge	30.08	http://www.neutrons.ornl.gov/users/proposal-calls
DESY	tba (typically 01.03 01.09)	https://photon-science.desy.de/users_area/calls__deadlines/index_eng.html

Institutional members and supporting institutions

Corporate members



Supporting institutions

(If you would like to see your logo here, please contact our treasurer)

Become a member of SGK/SSCr

Become a member

- ✓ Connect with researchers, scientists, and students from across scientific fields.
- ✓ Take part in events organized by the society.
- ✓ Drive the future activities of the society.
- ✓ Benefit from travel grants and PhD awards.
- ✓ Benefit from a network providing access to new collaborations and infrastructure.
- ✓ Stay up to date on upcoming events.

For more information as well as online registration, please go to our website https://swiss-crystallography.ch/en/membership
The yearly membership fee is CHF 40 for regular members and CHF 10 for students
SGK/SSCr is a member of the Swiss Academy of Science.

Connect with us:

Web: swiss-crystallography.ch
E-mail: swiss.crystallography@gmail.com
Twitter: Swisscrystallog

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Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

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