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

Sektion für Kristallwachstum und Kristalltechnologie
Section de Croissance et Technologie des Cristaux

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SGK / SSCr NEWSLETTER

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In this issue:

On the cover:
Collage of the various topics covered by the Swiss crystallographic community

The President's Page

Dear Members of the Swiss Society for Crystallography,

The challenge to work under COVID-19 pandemic conditions continues to impact on our private and professional lives. However, we have become familiar with the 'online world' for scientific exchanges and teaching and realized that some of these tools are extremely efficient and can speed-up processes and will to some extent also be kept in the post-corona era, which, we all hope, will start soon.

Online meetings, such as conferences, workshops and teaching events, have also allowed us to reach a broader audience, which brings new colors into our scientific exchanges. I repeat here the sentiment of our IUCr president Prof. Sven Lidin that I'm continuously impressed by people being smart, resourceful and innovative, but mention also the enormous enthusiasm reaching the community through online-conferences I have participated over the last year.

We see that structural sciences play a central role with increasing importance with respect to the understanding of the COVID-19 virus with its modifications and in the development of drugs and vaccines. We started our SSCr lectures in February with Dr. Andrea Thorn speaking about 'The Corona Structural Taskforce' and continue with our 2021 'Howard Flack Crystallography Lecture Series', which this year highlights structural biology in Switzerland. The program spreads over the spring and fall semesters and integrates six speakers from renowned Swiss labs; the agenda and registration access is given in this newsletter.

At the same time I'm happy to present in this edition of our newsletter the landscape of crystallography and structural sciences in Switzerland. Thank you for contributing and being part of this community!

In September 2020, we had our annual assembly in a ZOOM format and informed members about current actions and projects. Thank you for joining this reduced format of our SSCr Annual Meeting! This year on the 2nd of September 2021 we will hold our Annual Meeting at the Department of Chemistry, University of Fribourg. The theme will be 'From molecules to nanoparticles in Biology, Chemistry, Physics and Geology'. I invite especially our young crystallographers to present their research and to exchange ideas on this platform. Please submit your abstracts!

This year, the SSCr will award again the prize for the best PhD thesis in crystallography. We are waiting for your applications until the 31st of May 2021!

I wish you a safe time and take care.

Antonia Neels

President of the SGK-SSCr

Swiss Society for Crystallography

Howard Flack
Crystallographic Lectures Series

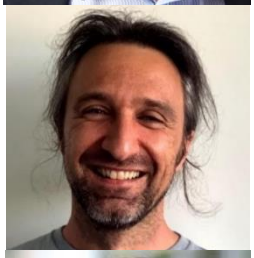
On the Topic:

'Structural Biology in Switzerland'

Organized as ZOOM lectures by the Empa Academy:
www.empa-akademie.ch/hfc-lecture

15.3.2021, 4-5pm
Prof. Gebhard Schertler
'SwissFEL adventures in room-temperature crystallography: From the structure of vertebrate and invertebrate rhodopsins to new applications in optogenetics'

12.4.2021, 4-5pm
Prof. Stefan Salentinig, University of Fribourg
'Bioinspired materials for functional foods'



18.5.2021, 4-5pm
Prof. Dimitrios Fotiadis, University of Bern
'Role of water molecules and networks in ligand binding and oligomerisation of the bacterial extreme acid resistance system transporter AdiC'

13.9. 2021, 4-5pm
Prof. Michael Hothorn, University of Geneva
'Plant signal transduction cascades – from atoms to phenotypes and back'

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 humour. The Swiss Society for Crystallography is proud to name an award and lecture series in his honour.

SGK-SSCr 2021
SGK-SSCr 2021

UNIVERSITÉ DE FRIBOURG
UNIVERSITÄT FREIBURG

Swiss Crystallographic Association,
Annual Meeting 2021

Department of Chemistry; University of Fribourg; Chemin du musée, 9; 1700 Fribourg

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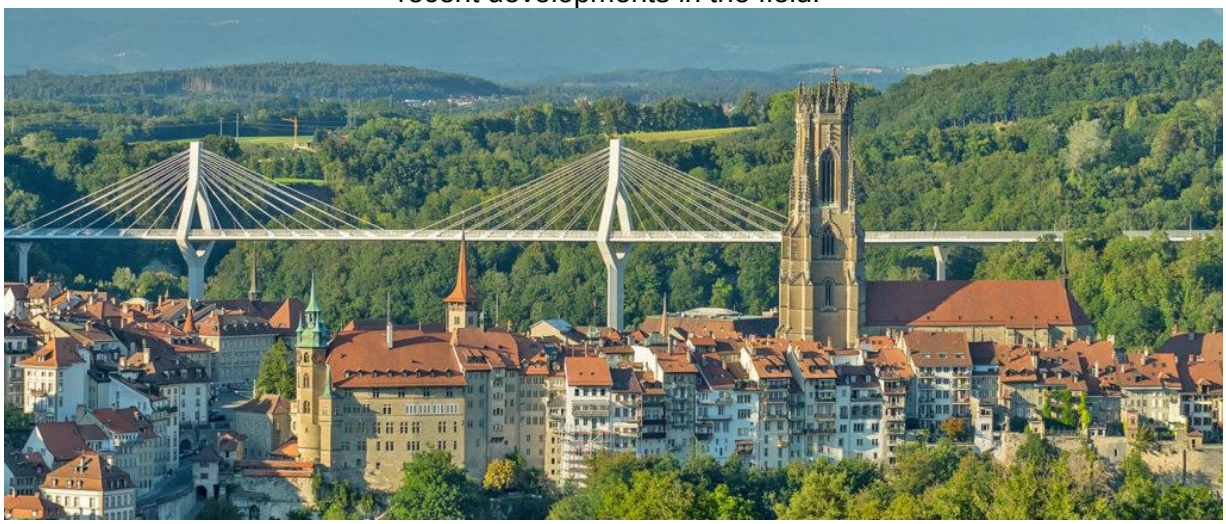
The 2021 annual meeting of the SGK/SSCr and general assembly will take place at the department of chemistry, University of Fribourg on Thursday 2nd of September 2021.

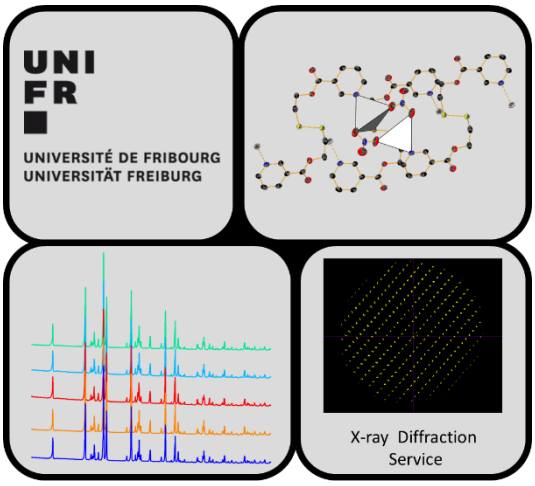
Invited speakers from academia, selected oral presentations and a poster session will show recent developments in the field.



The meeting is free of charge however please register by email to:
aurelien.crochet@unifr.ch before the 01.08.2021.
It's the occasion to present your work with an oral presentation (15 min) or/and with a poster.
Send us your abstract, please use the following template.

See you soon in Fribourg

Survey of the research groups/companies active in crystallography



X-ray diffraction Service

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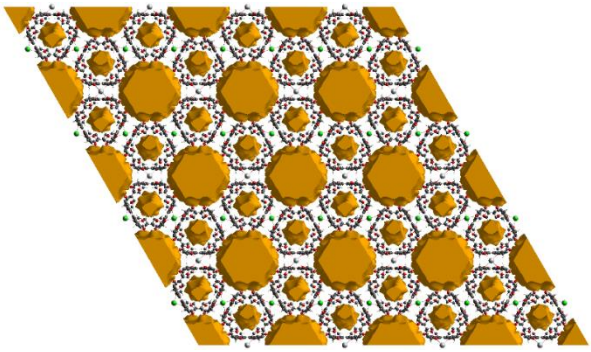
https://www.unifr.ch/chem/en/services/platforms/x-ray.html

The X-ray diffraction service of the Chemistry department of the University of Fribourg, built up by Prof. K. M. Fromm since 2006, is equipped with different single-crystal diffractometers (Mo, Cu and Ag radiation) and one powder diffractometer (Cu-$K\alpha_1$radiation). Dr. Aurélien Crochet is in charge of the service, provides single crystal structure determination service and assistance for the use of the powder diffractometer.



Crystal structure of a MOF with two pores sizes

The application field of the service is directly related with the research field of the customers. Among them are for example the investigation of the photolysis mechanism of nitroaromatic esters,[1] the structure of polyaramide hollow helices,[2] structure-property relationships of molecular sensors[3] and antimicrobial, silver-based compounds,[3] the study of precursors for oxide-materials[3] and the investigation of metal-organic frameworks for sensing purposes[3] or solid-state electrolytes for (high-voltage) batteries.[3] Covalent organic frameworks,[4] porous polymers[4] and rhenium dicarbonyl complexes[5] are further examples of research conducted in the department, using X-ray crystallography. Apart from these internal collaborations, the Crystallography lab offers its services also to research groups and industries at national and international level.

Recent publications and highlights:

K. Schindler, A. Crochet, F. Zobi; *RSC Adv.*, **2021**, *11*, 7511-7520; A. Finelli, S.-L. Abram, N. Hérault, A. Crochet, and K M. Fromm; *Cryst. Growth Des.*, **2020** *20* (8), 4945-4958; D. Yordanov, V. Deneva, A. Georgiev, A. Crochet, K. M. Fromm, L. Antonov; *Spectroch. Act. Part A*, **2020**, *237*, 118416

[1] Group of Prof. C. Bochet; [2] Group of Prof. A. Kilbinger; [3] Group of Prof. K. M. Fromm, [4] Group of Prof. A. Coskun; [5] Group of Prof. F. Zobi. For more information on these groups: https://www.unifr.ch/chem/en/

Crystallography at the Swiss Light Source:

The Materials Science beamline

The Swiss Light Source is a 2.4 GeV synchrotron located at the Paul Scherrer Institute, along the Aare near Villigen AG. Alongside beamlines devoted mostly to X-ray spectroscopy and imaging, it contains also some top class crystallographic beamlines. The PX-I, II, III are devoted to protein crystallography, being consistently at the world top, and the X04SA-Materials Science takes on the vast domain of crystallography, with excellence as beacon.

The Materials Science X04SA-MS beamline is permanently staffed by scientists Nicola Casati and Antonio Cervellino. It encompasses all the flavors of crystallography. Created as a shared-beam **X-ray powder diffraction** (XRPD) and surface diffraction beamline in the early 2000s, it has later been expanded to encompass **single crystal XRD**, **Total Scattering** and limited SAXS capabilities. It is also pioneering **time-resolved XRPD** up to several tens of kHz. It is equipped with many **state of the art detectors**. The MS has always been the testbed of the Mythen family of large-arc microstrip detector, since the first Mythen prototype in the mid-2000s. Then it has been exceptionally well served for 12 years by the Mythen II, with over 60000 channels spanning 120 degrees with 0.0036 degrees resolution, just replaced by a more performing Mythen III (now teething up). The Mythen detector has enabled **Total Scattering** experiments with unrivaled quality, due to its excellent intrinsic quality and the large angular coverage allowing medium energy experiments. Reciprocal space Total Scattering data analysis (DSE) has been pioneered here, ideally complementing the usual direct-space (PDF) approach. A large Pilatus 6M for frontal acquisitions complements ideally the microstrip – enabling also single crystal experiments - as well as an Eiger 1M ultrafast area detector for sub-ms time-resolved studies.

Ancillary sample environments are available for many of the most frequent sample conditioning needs. Temperatures from 4K to about 1800 K can be covered by different devices for capillary type samples. Gas lines to the diffractometer are installed to provide H_2, CO, CO_2, CH_4, O_2 and inert gas or their mixtures up to 100 bar. DAC cells for high pressure, an original in-situ ball milling device, a potentiostat for in situ battery cycling as well; consult the beamline staff.

User developed environments are often brought and installed at the beamline for specific experimental needs. Practically everything (where xrays have an entrance and exit path) can be installed. Special adaptations can be fabricated in most cases.

Experimental access. The bulk of beamtime is devoted to serving the international scientific community. Beamtime requests can be submitted in the form of scientific proposals. There are two deadlines per year (March 15 and September 15) for proposals concerning the X04SA-MS beamline only, and a supplementary one in February for combined X-ray and neutron diffraction experiments, in cooperation with the DMC and HRPT beamlines at the SINQ neutron source, also within the Paul Scherrer Institute. Moreover, RT XRPD experiments involving a few capillaries can be proposed at any time via the Mesquik rapid access channel.

Industrial service. Another large beamtime fraction is reserved for proprietary/industrial research, either via the Anaxam centre, via the PSI spin-off company Excelsus, specialized in pharmaceutical applications, or directly with our staff. The successful partnerships with companies is reflected in more than 10% of the beamtime being booked through this channel.

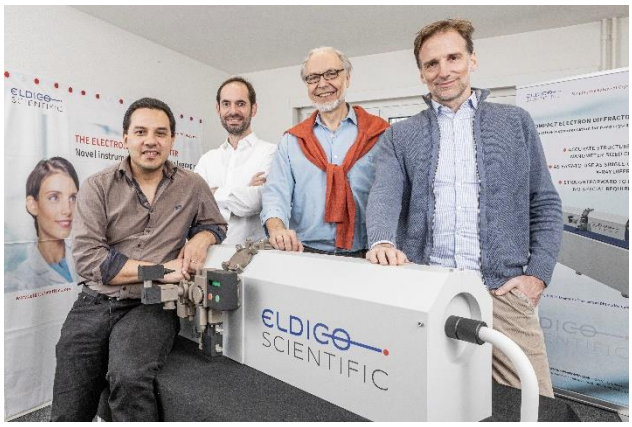


Figure 1: The four founders, from left to right: Gustavo Santiso-Q., Nils Gebhardt, Eric Hovestrevdt and Gunther Steinfeld.

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Website: www.eldico-scientific.com

ELDICO, a hardware company, was founded in June 2019 with the aim of filling a gap in the market: a *dedicated instrument* to determine the three-dimensional structures of nanoscale materials through electron diffraction.

3D-Electron Diffraction (3D-ED) has been gaining a lot of momentum in the recent years as it is a very powerful tool for the structural elucidation of nanocrystalline particles. After securing a *Science* nomination as “Breakthrough of the year 2018”, 3D-ED started to attract attention in various fields of research. Pioneers of the technique and researchers of other areas alike agree that the emergence of a dedicated device for 3D-ED would drive to unmapped territories in the research capabilities, solving thus structures of crystals that are too small for traditional approaches.


Angewandte International Edition Chemie
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Rapid Structure Determination of Microcrystalline Molecular Compounds Using Electron Diffraction

Dr. Tim Gruene, Julian T. C. Wennmacher, Dr. Christan Zaubitzer, Dr. Julian J. Holstein, Jonas Heidler, Ariane Fecteau-Lefebvre, Dr. Sacha De Carlo, Dr. Elisabeth Müller, Dr. Kenneth N. Goldie, Irene Regeni, Teng Li, Dr. Gustavo Santiso-Quinones, Dr. Gunther Steinfeld, Dr. Stephan Handschin, Eric van Genderen, Prof. Dr. Jeroen A. van Bokhoven, Prof. Dr. Guido H. Clever, Dr. Radosav Pantelic

First published: 16 October 2018 | https://doi.org/10.1002/anie.201811318 | Cited by: 15

Figure 2: The electron diffraction Breakthrough paper

Since its founding, with the fully committed activity of Gustavo Santiso-Quinones, Gunther Steinfeld, Eric Hovestreydt and Nils Gebhardt, ELDICO has been an advocate for an improved approach to nanoscale research. The company roots in Paul Scherrer Institute and maintains strong collaboration with innovation hubs from Switzerland. Moreover, ELDICO is at the fore-front of research on the novel technique and creates scientific communication opportunities through papers, presentations and, recently, taking crystal samples for measurement to prove once more that a concept has transformed in a powerful nano-analytical device. Drop us an email to find out more about your yet unsolved powders and what 3D-ED and ELDICO can do.

Recent publications and highlights:

[1] Santiso-Q., Gustavo, ‘What are Electron Diffraction and Nano-crystallography and why are they so important for scientists, researchers and industry?’
[2] Andrusenko et al, ‘Can ED distinguish between carbon and nitrogen atoms? What about the protons? Experiments on [2H]-3-amino-1,2,4 triazole.’
[3] Steinfeld & Santiso-Q., ‘The importance of Structural Elucidation in pandemics like COVID-19’
[4] Le Temps: Avec la nanocristallographie, une révolution est en vue

Figure 3: CXA Team with A. Neels, A. Borzì, M. Liebi, R. Zboray, A. Parrilli, S. Dolabella, N. Iranpour, L. Krupnik, S. Saghamanesh, A. Flisch, T. Kramer, I. Collings, A. Maurya, T. Lüthi, J. Hofmann, A. Dommann (from the upper left to the lower right).

Empa
Materials Science and Technology

Center for X-ray Analytics (CXA)
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Website:
http://www.empa.ch/x-ray

Empa's Center for X-ray Analytics enforces X-ray analytical method developments for materials science and technologies supporting Swiss and European research and industrial innovation. The development of new materials is connected to the possibilities for a comprehensive analysis of their structural and functional properties. Analytical methods do not only provide knowledge about the materials, but also support understanding of the production and aging process of these materials.
In one laboratory, we combine X-ray diffraction, scattering and imaging expertise going from the Ångström to the meter scale. At Empa we profit from the interface with materials research groups for the study of the structure – function relationship.

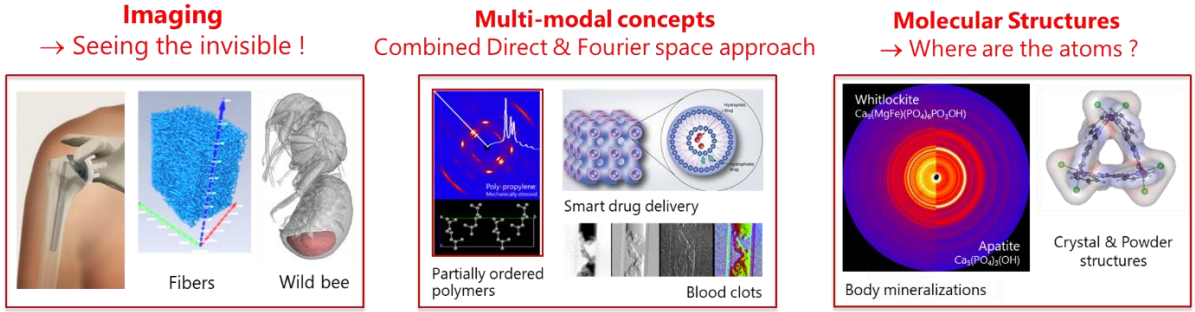

Figure 4: X-ray analytical and imaging concepts for understanding materials structure in health and materials science.

We develop multi-modal and multi-scale X-ray analytical methods for digital pathology based on data fusion algorithms to enable and improve diagnostics for precision medicine in collaboration with hospitals. In-situ techniques, especially microfluidics, are fostered for the understanding of the dynamics of systems [1]. In this context, X-ray imaging related topics are coupled with SAXS for the study of order-disorder structures in hierarchical systems [2]. We concentrate on high spatial resolution [3] for biological materials and dynamical studies for partially ordered material systems such as body mineralization's and polymers and nanoparticles in drug delivery systems.

[1] N. Iranpour Anaraki, A. Sadeghpour, K. Iranshahi, C. Toncelli, U. Cendrowska, F. Stellacci, A. Dommann, P. Wick, A. Neels, *Nano Research*, **2020**, 13(10), 2847-2856.
[2] A. Rodriguez-Palomo, V. Lutz-Bueno, X. Cao, R. Kádár, M. Andersson, M. Liebi, *Small*, **2021**, 2006229, 1-10.
[3] R. Zboray, *J. Microscopy*, **2021**,1–13.

Figure 5: The Biocolloids team with Stefan Salentinig, Rafael Freire, Marco Manca, Parth Kadakia, Matteo Frigerio, Linda Hong, Meron Debas, Bettina Tran, Andrea Lassenberger, Mark *Gontsarik and Samuel Watts (from top left).*

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The Biocolloids group at the Department of Chemistry at the University of Fribourg aims at understanding some of the fundamental principles in colloid and interface chemistry related to biological systems. Our research interests include directed self-assembly processes for the bottom-up creation of new nanomaterials, the design of functional surfaces, and programmable bio-nanointerfaces. Ultimately, we envision novel multi-functional materials with a broad impact in fields including food science and MedTech. Towards this goal, we study the composition-structure-activity relationships of nature's own materials and interfaces to unravel original mechanisms at play that have been optimized by evolution over millions of years.

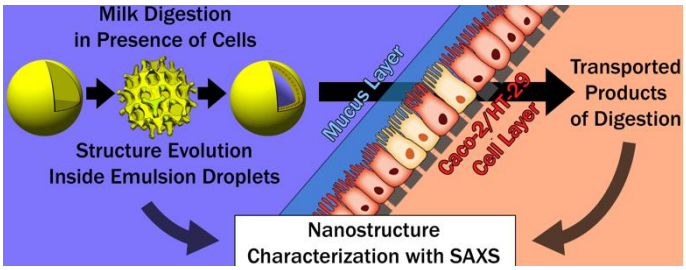

Figure 6: In-situ synchrotron SAXS study of formation during the digestion of milk in the presence of a cell culture model simulating the small intestine.[1]

We are highly active in the adaption and integration of *in situ* X-ray scattering and diffraction platforms for characterization. Highlights are:

(i) dynamic flow-through SAXS / WAXS set-ups to study liquid crystallization during emulsion digestion;
(ii) *in situ* GI-SAXS / WAXS platforms to study the response of (liquid) crystalline films to changes in environmental conditions;
(iii) 2-dimensional X-ray scattering techniques to analyze partially ordered systems in the bulk and on surfaces.

We combine these methods with numerical data analysis as well as chemical and biological studies to advance the understanding and the comprehensive design of material interactions across boundaries - on the molecular, structural and the functional level. [1-3] One recent example is our discovery of liquid crystalline structure formation during the digestion of milk to deliver nutrients and trigger cells interactions that can guide the design of advanced food and drug delivery materials (Fig. 2).[1]

Recent publications and highlights:

[1] C. Hempt, M. Gontsarik, T. Thurnherr, C. Hirsch, S. Salentinig, JCIS, 2020, 574, 430-440.
[2] S. Watts, T. Julian, K. Maniura, T. Graule, S. Salentinig, ACS Nano 2020, 14, 1879-1887.
[3] O. Glatter, S. Salentinig, COCIS, 49, 2020, 82-93.

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https://chemie.unibas.ch/en/department/services/x-ray-analyses/

Figure 7: Dr. Alessandro

The crystallography lab in the Chemistry Department of the University of Basel is run by me, Alessandro Prescimone. I started in 2014 alongside Markus Neuburger and I am the sole holder of the position since since the middle of 2018. The lab provides a service for the research groups of the Chemistry Department including practical and theoretical crystallographic training for PhD students and Postdocs. High Pressure single crystal diffraction is also offered with experiments performed at the Diamond Light Source Synchrotron in UK. The work focusses mostly on organic and metallo-organic samples. The lab has one STOE Stadi-P powder diffractometer, an old Bruker Apex II single crystal instrument and as crystals are getting smaller and smaller we are very happy that we can also count on our STADIVARI diffractometer with a Metaljet source and a Pilatus R3 detector, as depicted in figure 2. Now that all the "Prima Donna" issues have been dealt with and solved, this is finally a more "mature" instrument that allows us to measure extremely small samples producing data of outstanding quality (assuming there is enough crystallinity in the sample, of course).

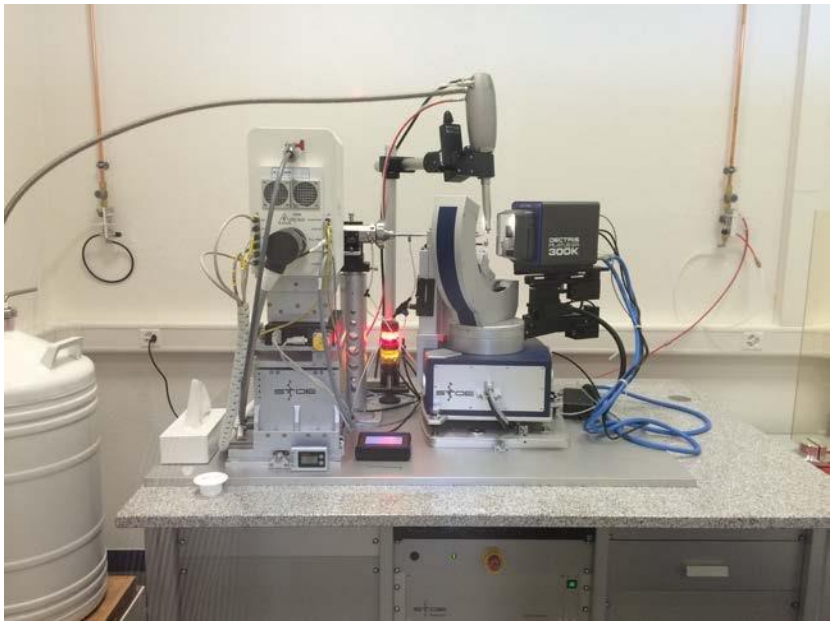

Figure 8: Our STADIVARI with Metaljet generator and Pilatus detector.

Dr. Alessandro Prescimone

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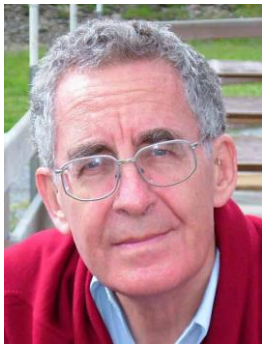
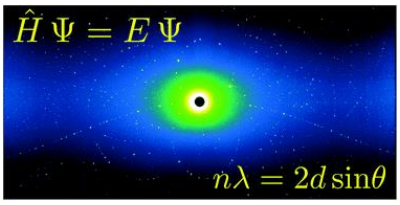
www.chem.uzh.ch/en/research/groups/linden/buergi.html

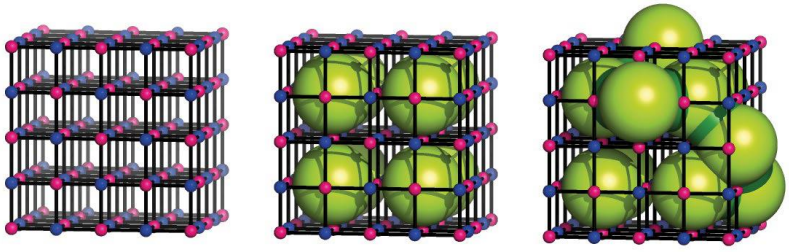


Hans-Beat Bürgi is a permanent academic guest at the Chemistry Department of the University of Zürich, Professor Emeritus at the University of Berne, Switzerland, and a co-director with Prof. Anthony Linden of the *Zurich School of Crystallography* [1], a two-week intense course for international students, which was inaugurated in 2007. His research interests include:



- *Quantum Crystallography*: By combining diffraction experiments with quantum chemical calculations the scope of X-ray crystal structure determination is extended. Hirshfeld atom refinement (HAR) provides accurate anharmonic ADPs, hydrogen atom positions and their ADPs [2]. This work is a collaboration with Dylan Jayatilaka at the University of Western Australia and Simon Grabowsky at the University of Berne.

- *Analyzing diffuse scattering* [3]: Interesting properties of many crystalline materials result from packing faults. Such faults may be studied from disorder diffuse scattering [3] and multi-temperature Bragg diffraction [4]. The resulting diffuse scattering is interpreted in terms of atomistic models with 3D-PDF methods, Monte Carlo calculations and genetic algorithms. These studies are collaborations with Andrew Goodwin at the University of Oxford and Omar Yaghi at UC Berkeley.



Prussian Blue Analogs and ordered or disordered vacancies (green)
$M^{II}[M'^{IV}(CN)_6]_1$ $M^{III}[M'^{II}(CN)_6]_{3/4}\square_{1/4}$ $M^{II}[M'^{III}(CN)_6]_{2/3}\square_{1/3}$

[1] https://www.chem.uzh.ch/linden/zsc/
[2] S. Grabowsky, A. Genoni, H.-B. Bürgi, Quantum crystallography, *Chem. Sci.*, ***8***, 4159-4176, **2017**, DOI: 10.1039/c6sc05504d
[3] Simonov, A., De Baerdemaeker, T., Bostrom, H.L.B., Gomez, M.L.R., Gray, H.J., Chernyshov, D., Bosak, A., Bürgi, H.-B., Goodwin, A.L., Hidden diversity of vacancy networks in Prussian blue analogues, *Nature 578*, 256, **2020**
[4] S. Lee, H.-B. Bürgi, S. A. Alshmimri, O. M. Yaghi, Impact of Disordered Guest−Framework Interactions on the Crystallography of Metal−Organic Frameworks, *J. Am. Chem. Soc*. *140*, 8958−8964, **2018**

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Radovan Černý

Figure 9: The crystallography group at University of Geneva.

The Laboratory of Crystallography at the University of Geneva is a part of the Dpt. of Quantum Matter Physics, Faculty of Sciences. The laboratory awards a Ph.D. degree in crystallography, teach the crystallography for students in physics and bio-chemistry, and in collaboration with the Section of Chemistry provides the crystallographic service. The laboratory was created in 1970 as the first Chair of Crystallography in the French-speaking Switzerland. The actual research directions are in the field of crystallography based design of light metal hydrides [1] as solid electrolytes in Li- and Na-batteries [2,3] (group of R. Černý), in collaboration with the Section of Chemistry on spin crossover materials and rare earths based coordination polymers (C. Besnard, L. Guénée) and in collaboration with MPDS in the development of Pearson's Crystal Database (R. Turdean). It is also the place where the computer program Fox [4] has been created, and the improvement of methods for crystal structure solution stays one of the important activities. In the past, the laboratory worked also in the field of crystallography and crystal chemistry of inorganic compounds (E. Parthé), and of intermetallics and their properties such as hydrogen storage, magnetism and supraconductivity (K. Yvon, R. Černý). The methods of structure solution from single crystal data, especially the absolute structure determination, have been another important contribution of the laboratory (H. Flack, G. Bernardinelli).

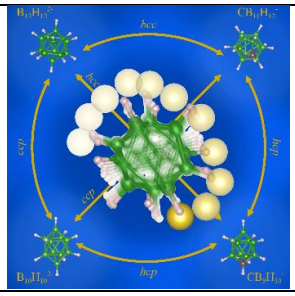

Figure 2: Structures of hydroborate polyanions $[CB9H10]^-$, $[B10H10]^{2-}$, $[CB11H12]^-$, and $[B12H12]^{2-}$. Arrows indicate the anionic mixture and resulting anion sublattice packing in sodium solid electrolytes [3].

Recent publications and highlights:

[1] The Crystal Chemistry of Inorganic Hydroborates (dedicated to Howard Flack). *Chemistry* (2020), 2(4), 805-826, doi.org/10.3390/chemistry2040053
[2] Room-temperature-operating Na-ion solid state-battery with complex hydride as electrolyte. *Electrochem. Comm.* (2019), 106, 106534, doi.org/10.1016/j.elecom.2019.106534
[3] Closo-Hydroborate Sodium Salts as an Emerging Class of Room-Temperature Solid Electrolytes. *Cell Reports Phys. Sci.* (2020), 1, 100217, doi.org/10.1016/j.xcrp.2020.100217
[4] Program Fox: http://fox.vincefn.net/

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Figure 10: The Spingler group in Fall

In recent years, the Spingler group has continued to develop methods for growing single crystals.[1] We have succeeded in designing a small molecule anion screen, which efficiently allows the crystallization of water soluble cations.[2] The screen contains 77 different anions and has been commercialized. With this screen we could show that robots can help also chemists to crystallize interesting molecular salts, including active pharmaceutical ingredients (API). We have extended the use of that screen to the so-called under-oil crystallization method, which does not require the usage of an expensive pipetting robot.[3] The crystal structure of a difficult to crystallize photosensitizer for photodynamic therapy, shown in Figure 2, was grown with help of this under-oil method.[4] Finally, we have used our anion screen to crystallize coordination complexes.[5]

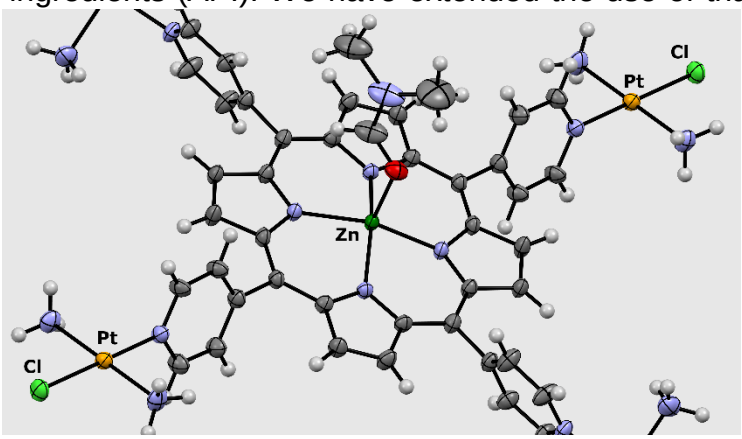

Figure 11: Crystal structure of a platinated porphyrin [4], which was crystallized employing the under-oil technique **[3].**

Recent publications and highlights:

[1] P. P. Nievergelt, B. Spingler, *CrystEngComm* **2017**, *19*, 142.
[2] P. P. Nievergelt, M. Babor, J. Čejka, B. Spingler, *Chem. Sci.* **2018**, *9*, 3716.
[3] M. Babor, P. P. Nievergelt, J. Čejka, V. Zvoníček, B. Spingler, *IUCrJ* **2019**, *6*, 145.
[4] R. Rubbiani, W. Wu, A. Naik, M. Larocca, L. Schneider, R. Padrutt, V. Babu, C. König, D. Hinger, C. Maake, G. Gasser, S. Ferrari, B. Spingler, *Chem. Commun.* **2020**, *56*, 14373.
[5] R. Alvarez, P. P. Nievergelt, E. Slyshkina, P. Müller, R. Alberto, B. Spingler, *Dalton Trans.* **2020**, *49*, 9632.

Figure 12: LMTM members. Prof. Roland Logé and his team.

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The research activities at LMTM relate to processing and manufacturing of metals and alloys in the solid state, focusing on the ability to tailor microstructures, and the associated material properties. Topics of interest include recrystallization, phase transformations, precipitation, grain growth, textures and grain boundary engineering, internal stresses and cracking phenomena, with applications to bulk metal forming and laser based additive manufacturing. An in-house Laser Powder Bed Fusion (LPBF) platform promotes further development of the process, and the enhanced control of microstructures.

LMTM is equipped with Scanning Electron Microscopes (SEM, Electron BackScatter Diffraction (EBSD) and Transmission Kikuchi Diffraction (TKD) systems. We are particularly invoved in the experimental and theoretical studies of the crystallography of martensitic phase transformations and growth and deformation twinning in metals, alloys and minerals. Our last contributions were obtained on the concepts of variants and twins, and on new algorithms of lattice reduction and hyperplanar projection in N dimensions.

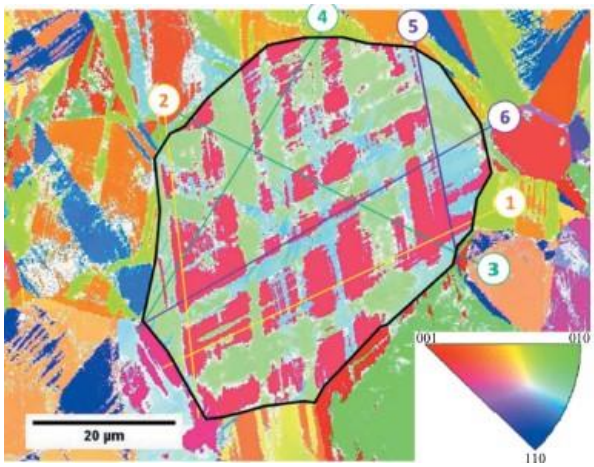

Figure 13: EBSD map of the tetragonal martensite in a red gold (Au-Cu) alloy. From Ref[2].

Recent publications and highlights:

[1] C. Cayron (2020) *What EBSD and TKD Tell Us about the Crystallography of the Martensitic B2-B19' Transformation in NiTi Shape Memory Alloys*. Crystals 10, 562.
[2] M. N. D. Larcher; C. Cayron; A. Blatter; R. Soulignac; R. E. Logé (2019) *Electron backscatter diffraction study of variant selection during ordering phase transformation in L1(0)-type red gold alloy*. J. Appl. Cryst. (2019). 52, 1202.
[3] C. Cayron (2019) *The transformation matrices (distortion, orientation, correspondence), their continuous forms and their variants.* Acta Cryst. (2019). A75, 411.

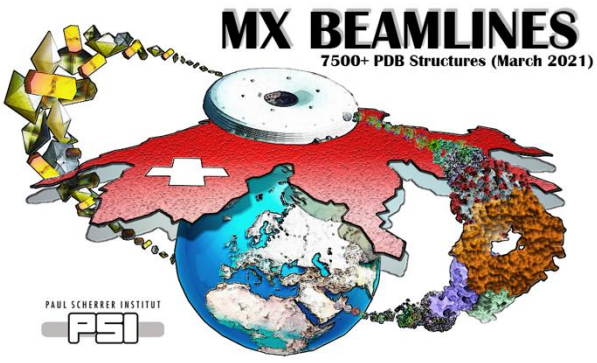

Figure 14: The macromolecular crystallography at SLS (see our website for names of the group members and their profiles)

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Website:
https://www.psi.ch/en/macromolecular-crystallography

The macromolecular crystallography (MX) group was established to build and operate protein crystallography (PX) beamlines and develop synchrotron-based MX methods at the Swiss Light Source in 1999. In the past two decades, we have developed three high-performance and productive PX beamlines and one crystallization facility that have attracted thousands of users from academic institutions and the pharmaceutical industry in Switzerland and abroad. Together, our users have produced some 4,000 publications and 7,500 protein structures. We have pioneered some key beamline instrumentation like micro-focus optics, pixel-array detectors, and multi-axis goniometry. These developments have spurred the advance of novel MX methods such as native-SAD phasing, serial synchrotron crystallography, and time-resolved crystallography. In addition, the MX group has actively collaborated with external groups on complex structural biology projects, including the recent global effort on structure-based ligand screening against SARS-CoV-2 proteins.

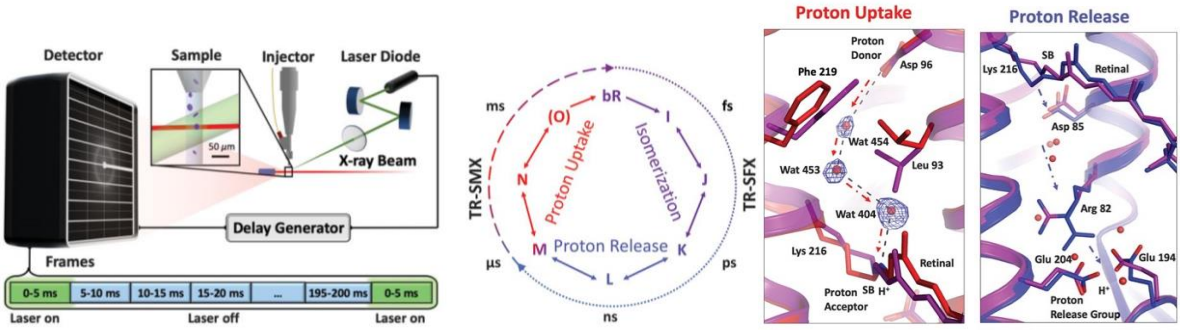

Figure 15: Proton uptake mechanism is revealed by time-resolved serial synchrotron

Recent publications and highlights:

[1] Weinert, T. *et al.* Fast native-SAD phasing for routine macromolecular structure determination. *Nat. Methods* **12**, 131–133 (2015).
[2] Leonarski, F. *et al.* Fast and accurate data collection for macromolecular crystallography using the JUNGFRAU detector. *Nat. Methods* **15**, 799–804 (2018).
[3] Huang, C.-Y. *et al.* In situ serial crystallography for rapid de novo membrane protein structure determination. *Commun Biol* **1**, 124 (2018).
[4] Weinert, T. *et al.* Proton uptake mechanism in bacteriorhodopsin captured by serial synchrotron crystallography. *Science* **365**, 61–65 (2019).

Figure 16: The facility team: Tony Linden, Olivier Blacque and Hans-Beat Bürgi.

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The X-ray Crystallography Facility of the Department of Chemistry at the University of Zurich is an analytical service laboratory which uses X-ray diffraction to determine the three-dimensional, single-crystal structures of small molecules, from organics through organometallic complexes to inorganic compounds. The laboratory provides rapid and high-quality structure analyses in support of the research projects of the members of the Department of Chemistry. We also collaborate with external academic and industrial clients. Equipment includes Rigaku Synergy-S and Super-Nova single crystal diffractometers, and a Rigaku SmartLab powder XRD instrument.

The group has a strong interest in crystallographic teaching [1]. Since 2007, we have been organising the popular Zurich School of Crystallography, which trains enthusiastic young crystallographers from around the world [2].

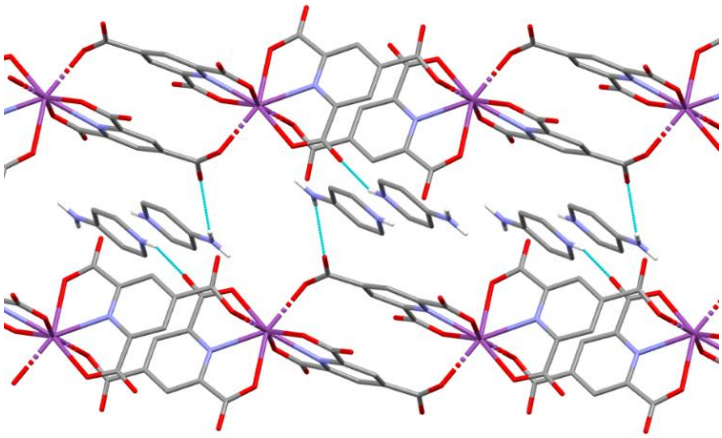

Figure 17: A Bi(III) coordination polymer with 2,4,6-pyridine-tricarboxyate [3].

Recent research has focused on:
– coordination polymers involving bismuth(III) (Fig. 2) [3] and how intermolecular interactions influence the supramolecular and structural properties of crystalline materials.
– disorder in MOFs [4] and in Prussian Blue Analogues [5].

Recent publications:

[1] A. Linden, Acta Crystallogr. **2020**, *E76*, 765–775.
[2] https://www.chem.uzh.ch/linden/zsc/
[3] L. Senior, A. Linden, Polyhedron, **2020**, *184*, 114564.
[4] S. Lee, H.-B. Bürgi, S.A. Alshmimri, O.M. Yaghi, J. Am. Chem. Soc. **2018**, *140*, 8958–8964.
[5] A. Simonov, T. De Baerdemaeker, H.L.B. Bostrom, M.L.R. Gomez, H.J. Gray, D. Chernyshov, A. Bosak, H.-B. Bürgi, A.L. Goodwin, Nature, **2020,** *578*, 256–260.

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*Figure 18: The work group of PD Dr. Simon Grabowsky (upper left) as of February 2021. Dr. Loraine Andrade Malaspina (upper right). Dr. Michał Andrzejewski (*lower left). Dr. Florian Kleemiß (lower right).

Our research group at the University of Bern develops quantum-crystallographic techniques for chemical-bonding analysis. In quantum crystallography, we use the cooperative effect of molecules periodically arranged in a crystal lattice like a magnifying glass to study quantum phenomena such as chemical bonding that could otherwise only be observed with an enormous technical effort or not at all. Software development accompanies method development in our group. We have, e.g., published the software *NoSpherA2* inside the widely used crystallographic refinement program *Olex2*. It allows the quantum-crystallographic refinement method Hirshfeld Atom Refinement (HAR) to be applied to a broad variety of crystal structures coming from routine X-ray diffraction experiments.[1]

Figure 2 shows an example where a bonding analysis based on quantum crystallography could experimentally contribute to a long-standing problem: hypervalency. In textbook chemistry, we still draw Lewis resonance structures of the oxyanions phosphate, sulfate or perchlorate that violate the octet rule at the central period-3 element. We could measure that in fact these structures have 0% contribution to the overall electronic state, whereas ionic and negatively hyperconjugated descriptions prevail.[2]

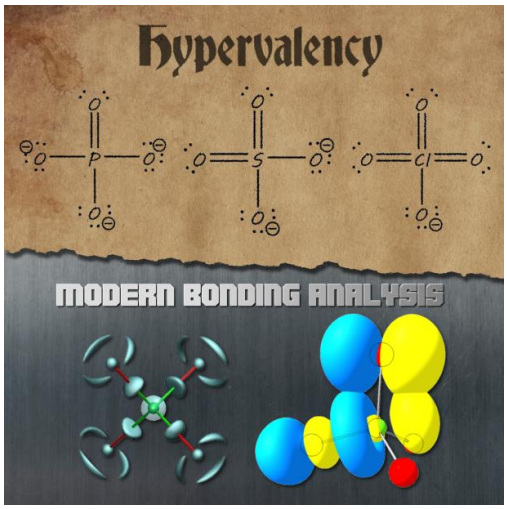
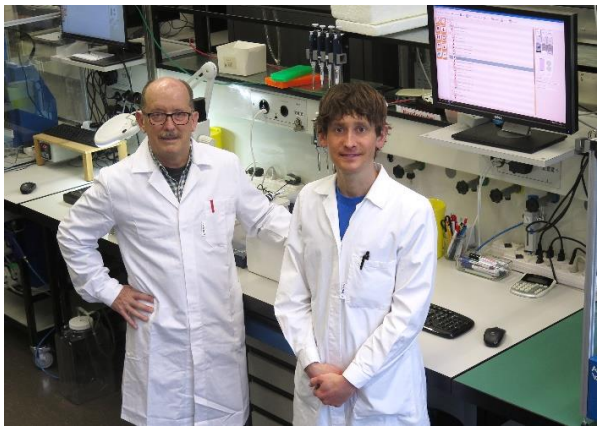


Figure 19: The discrepancy between historical bonding concepts such as hypervalency expressed with Lewis structures and modern bonding analysis based on quantum crystallography. Adapted from the cover of Chemistry – A European Journal (2019-25/26).[2]

[1] F. Kleemiss, O. V. Dolomanov, M. Bodensteiner, N. Peyerimhoff, L. Midgley, L. J. Bourhis, A. Genoni, L. A. Malaspina, D. Jayatilaka, J. L. Spencer, F. White, B. Grundkötter-Stock, S. Steinhauer, D. Lentz, H. Puschmann, S. Grabowsky, *Chem. Sci.* **2021**, *12*, 1675–1692.
[2] M. Fugel, L. A. Malaspina, R. Pal, S. P. Thomas, M. W. Shi, M. A. Spackman, K. Sugimoto, S. Grabowsky, *Chem. Eur. J.* **2019**, *25*, 6523 – 6532.



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The PCC Team Beat & Christoph Blattmann

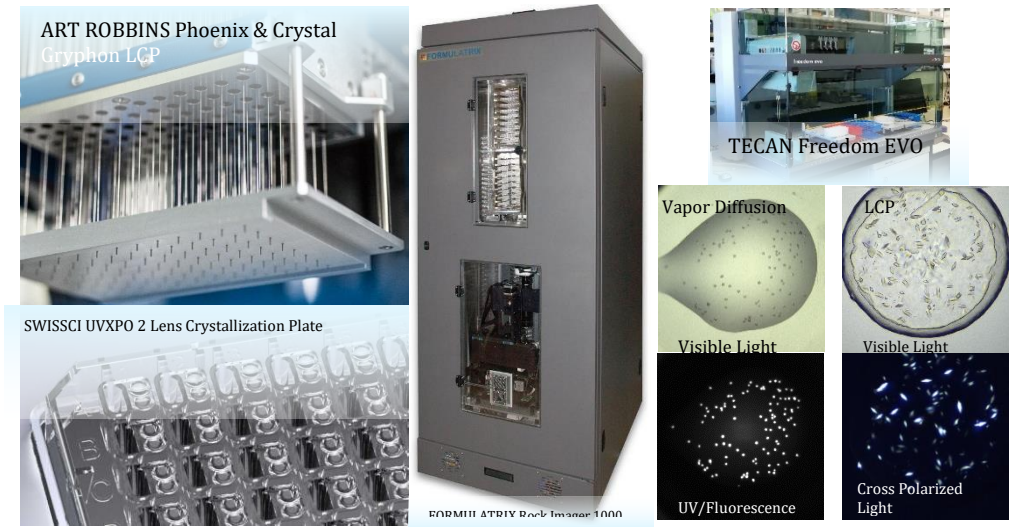
High-Throughput Protein Crystallization @ University of Zürich

The Protein Crystallization Center high-throughput screening lab at the University of Zürich – PCC@UZH – has been professionally assisting the academic and industrial research community to advance their research in structural biology for over 19 years. Just over the past year, more than thirty academic and industrial research groups took advantage of PCC's expertise in a wide range of crystallization techniques for soluble and membrane proteins, organic salts, complexes and pharmaceutical ingredients.

The experienced staff at PCC sets up the vapor diffusion and LCP crystallization experiments according to the researcher's specifications at 4° or 20°C at the nano-liter scale using automated liquid-handling robots. Thereafter, crystallization plates are incubated in one of the facility's two state-of-the-art Rock Imager 1000 (4°C or 20°C) specified by the researcher. The integrated visible (w/ & w/o cross polarizer) and UV/Fluorescent imaging systems from Formulatrix enable researchers to observe crystal formation remotely from their regular workspace. PCC additionally offers basic infrastructure and work space for fishing crystals.

With the "Freedom EVO" liquid handler from Tecan, PCC provides researchers with custom-prepared refinement screens composed with up to 30 different stock solutions. The versatile Excel screen-builder offered by PCC provides options to cover the varying needs within the research community. Quick and intuitive design of screens consisting of wells with constant constituent concentration, linear pH or concentration gradients across desired well ranges as well as selective constituent addition to particular wells lay within the realm of possibilities.

For more information contact the PCC@UZH team by email or go to our web site at:
https://www.bioc.uzh.ch/research/core-facilities/protein-crystallization-center/



Phase Solutions

Beyond your laboratory results

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High Throughput Protein Crystallization at PCC@UZH

Phase Solutions Sàrl was created by crystallographers of the Laboratory of Crystallography at EPFL (École Polytechnique Fédérale de Lausanne), Switzerland. It was founded by Prof. Gervais Chapuis with Dr Alla Arakcheeva as CEO and Dr Philip Pattison as Adviser. The company is closely collaborating with EPFL and other research institutions in Switzerland and abroad.

Phase Solutions (PS) provides crystallography research services including incommensurately and commensurately modulated structures, composites, phase transitions studies, nano-particle size estimations, impurity tests of amount smaller than 1%, structural defects, among others. PS also work with minimal amount of powder samples.

PS enables you to have access to top specialists in crystallography, the most advanced diffraction equipments and extended experience in the interpretation of X-ray results.

The following selection of published studies have been performed recently with PS assistance:

- **One-dimensional composite host–guest structure in $BaVS_3$** DOI 10.1107/S2052520620016108
- **High-Pressure Synthesis of Rare-Earth Borate-Nitrate Crystals for Second Harmonic Generation** DOI 10.1021/acs.inorgchem.0c0290
- **Preferential out-of-plane conduction and quasi-one-dimensional electronic states in layered 1T-TaS_2** DOI 10.1038/s41699-020-0145-z
- **Incommensurate crystal structure of $PbHfO_3$** DOI 10.1107/S205252061901494X
- **The influence of the incommensurately modulated structure on the physical properties of $Fe_{1.35}Ge$** DOI: 10.1016/j.jallcom.2019.04.159
- **Pressure-induced transformation of $CH_3NH_3PbI_3$: the role of the noble-gas pressure transmitting media** DOI: 10.1107/S2052520619004554
- **Effect of Thermal Cycling on the Structural Evolution of Methylammonium Lead Iodide Monitored around the Phase Transition Temperatures** DOI:10.1002/solr.201900044
- **$Sr_2Pt_{8-x}As$: a layered incommensurately modulated metal with saturated resistivity.** DOI: 10.1107/S2052252518007303
- **Influence of the organic cation disorder on photoconductivity in ethylenediammonium lead iodide, $NH_3CH_2CH_2NH_3PbI_4$.** (DOI: 10.1039/c8ce00259b)
- **High-pressure transformation of $MAPbI_3$: role of the noble-gas medium.** DOI: 10.1107/S2053273317081608
- **Controlling structural and magnetic properties of IONPs by aqueous synthesis for improved hyperthermia** DOI 10.1039/C7RA00687J
- **Optically switched magnetism in photovoltaic perovskite $CH_3NH_3(Mn:Pb)I_3$** DOI 10.1038/ncomms1340

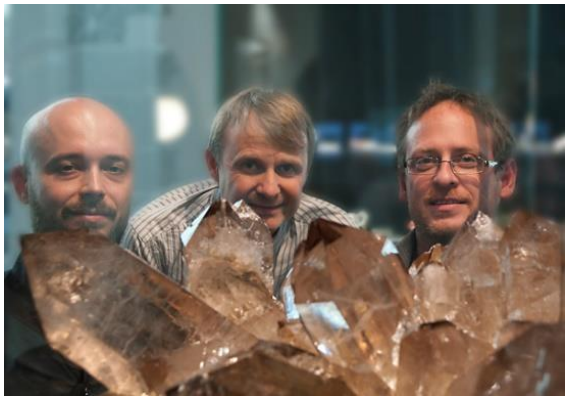

Figure 20: The SMoCC group Nils Trapp, Michael Wörle and Michael Solar (f.l.t.r)

SMoCC

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The Small Molecule Crystallography Center (SMoCC) is a technology platform of the Department for Chemistry and Applied Biosciences at the ETH Zurich. We support the research activities by providing facilities for various characterizations by X-ray diffraction techniques. A large fraction of our work comprises high throughput routine single crystal structure analysis. Moreover, in order to ensure maximum flexibility and to be able to solve challenging crystallographic problems, we grant a direct access to the instruments for interested (PhD-) students and postdocs after adequate training. We also offer support on crystallization techniques and problematic structures beyond simple routine structure analyses (charge density determinations, disorder and diffuse scattering, twin formation, incommensurate and modulated structures, phase transitions and in situ crystallizations). We are developing in house devices for crystallization and sample handling at non-ambient conditions (low temperature, inert conditions). Our platform includes also powder diffraction instruments and we perform routine phase identification (fingerprinting) as well as quantitative phase analysis and structure analysis on the basis of powder diffraction data (Rietveld refinements). As the National Affiliate Center of the Cambridge Crystallographic Data Centre we host and distribute the Cambridge Structure Database (CSD) to all academic institutions in Switzerland and also provide acces to the Inorganic Crystal Structure Data Base (ICSD).

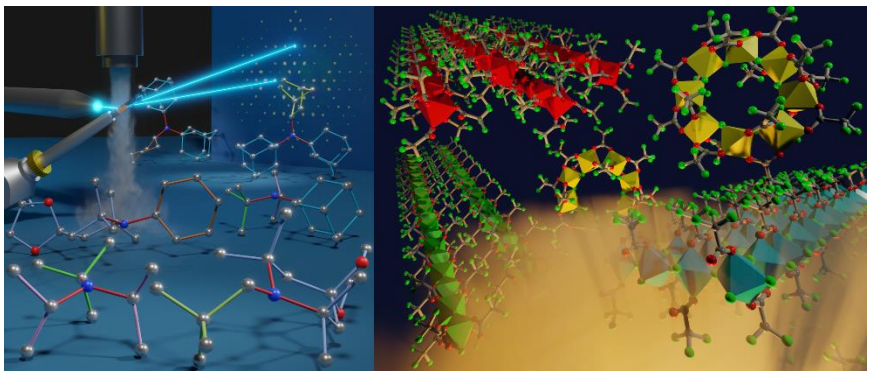

Figure 21: In-situ crystallization of liquids on the diffractometer in capillaries and subsequent measurement (left). Thermal decomposition of metal-trifluoroacetates and structural characterization of the intermediate products by powder and single-crystal diffraction (right).

Recent publications and highlights:

[1] M. Wörle, C.P. Guntlin, L. Gyr, M.T. Sougrati, C.-H. Lambert, K.V. Kravchyk, R. Zenobi, M.V. Kovalenko; *Chem. Mater.* **32** (2020), 2482-2488.
[2] K. Banert, M. Heck, A. Ihle, T. Shoker, M. Wörle, D. Boese; *Chem. Eur. J.*, **27** (2021), 3700-3707.
[3] C. Gropp, S. Fischer, T. Husch, N. Trapp, E. M. Carreira, F. Diederich, *J. Am. Chem. Soc.* **142**, (2020) 4749.

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https://www.empa.ch/econversion

Figure 22: Empa's laboratory "Materials for Energy

The laboratory *Materials for Energy Conversion* is a research laboratory at Empa, the Swiss Federal Laboratories for Materials Science and Technology, led by Dr. Corsin Battaglia. Competences range from the synthesis and characterization of battery materials and their integration in lab-scale prototype cells including next-generation lithium-ion battery cells and post-lithium-ion technologies (e.g. sodium batteries, batteries with metal anodes, cobalt-free cathodes, solid electrolytes, etc.) [1-4]. The lab disposes of an extensive infrastructure for materials synthesis and modification, slurry processing, electrode coating, cell assembly, and characterization of their structural, electrochemical, and thermal properties. It serves as the coordinator of the European project sense-battery.eu, and as Swiss representative and contact point for the large-scale European battery initiative battery2030.eu.

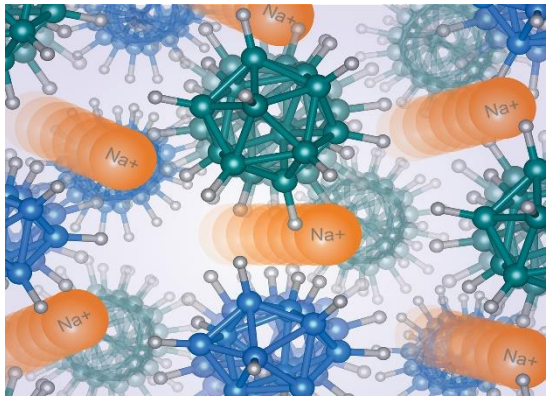
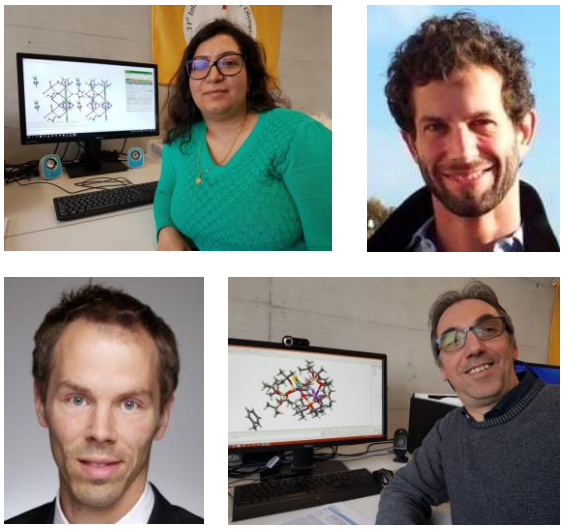


Figure 2: Schematic representation of the anion-assisted Na^+-conduction in a hydroborate

Solid electrolytes, which form the heart of a future all-solid-state battery, are a major research focus of our laboratory. We developped a new class of hydroborate-based electrolytes culminating in the realization of a 4 V all-solid-state sodium battery, stable for more than 800 cycles, using $Na_4(CB_{11}H_{12})_2(B_{12}H_{12})$ as electrolyte, combining high ionic conductivity > 1 mS cm^{-1} at room temperature, an electrochemical stability window of ~4 V, high thermal stability, and favorable mechanical properties [3]. Understanding the dynamic crystal structure of hydroborate solid electrolytes is key to understand and to taylor the ionic conductivity. In hydroborates, X-ray diffraction revealed a structure that offers rotational freedom to the anions, assisting the Na transport between partially occupied Na positions responsible for the high ionic conductivity as schematically represented in figure 2 [4-6].

Recent publications and highlights:

[1] M. C. Bay et al., *Adv. Energy Mater.* 2020, **10** (3), 1902899.
[2] D. Reber et al., *Adv. Energy Mater*. 2021, **11** (5), 2002913.
[3] R. Asakura et al., *Energy Environ. Sci.* 2020, **13** (12), 5048-5058.
[4] L. Duchêne et al., Chem. Mater. 2019, **31**, 3449-3460
[5] S. Payandeh et al., Chem. Mater. 2020, **32**, 1101-1110.
[6] S. Payandeh et al., *Adv. Funct. Mater*. 2021, 2010046



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https://www.epfl.ch/schools/sb/research/isic/platforms/x-ray-diffraction-and-surface-analytics

Figure 23: The team, Farzaneh Fadaei Tirani, Mounir Mensi, Pascal Schouwink and Rosario Scopelliti (l.t.r)

The X-ray diffraction and Surface Analytics Facility of the Institute of Chemical Sciences and Engineering is a central user facility at the EPF Lausanne. It was created in 2017 by merging different X-ray labs on the central campus in Lausanne and the EPFL Antenna EPFL Valais Wallis in Sion. The latter is part of the new campus "Energypolis", a joint venture between federal, cantonal and private institutions, focussing on energy-related materials science. This campus is currently in phase 2 expansion and very recently the University of Applied Sciences Western Switzerland - Valais (HES-SO Valais) has joined EPFL on the campus, and we look forward to welcoming them in our user labs. Next to different methodologies applying X-ray scattering (an X-ray structure service, 2 materials diffraction labs with equipment for non-ambient measurement conditions) our platform hosts instrumentation and expertise on surface investigations using spectroscopy and imaging. Frequent use is also made of setups at the Swiss Norwegian Beamlines of ESRF and the Materials Science beamline of PSI. Our ambition is to provide a comprehensive characterization of samples and devices on different length scales and under different environments, elucidating atomic, nanoscopic and electronic structure. Next to this our main mission is to support and educate a diverse and growing user pool of currently approximately 45 research groups, the entire instrument pool being fully open to internal as well as external users, with very few exceptions.

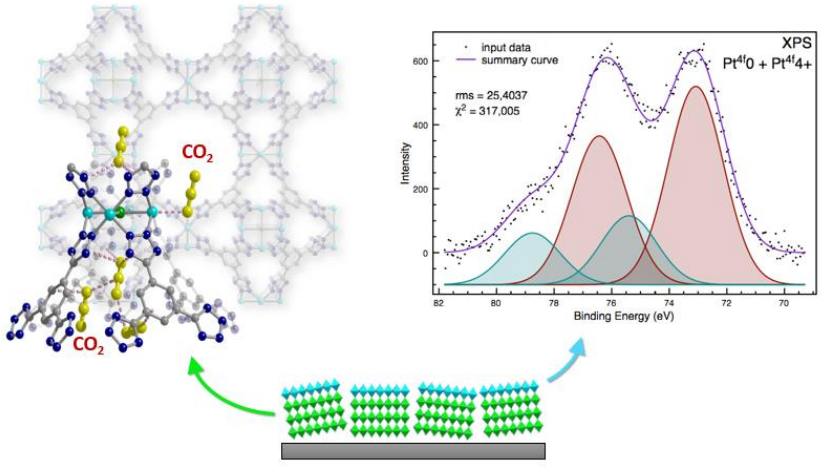

Figure 2: Surface and bulk, electronic and crystal structure.

The ESRF by night, SNBL group members: Charles McMonagle, Dragos Stoian, Dmitry Chernyshov, Francois Pegot, Hermann Emerich, Kenneth Marshall, Monique Faure, Vadim Diadkin and Wouter van Beek

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Website: http://www.snbl.eu

The mission of the SNBL is to provide scientists from Norway and Switzerland, from both academia and industry, with access to synchrotron radiation. Since 1996, SNBL is serving the Swiss community and has a large experience with complex crystallographic problems related to materials chemistry and physics. Novel materials come often at the expense unprecedented complexity where multi technique (in-situ or operando) experiments become vital for understanding their properties. SNBL is specialized in performing such experiments. Typical examples are on gas separation/storage frameworks, battery cycling, catalysts at work, nucleation and growth processes, strongly correlated systems at low-temperatures, domain wall motion of ferroelectric materials under electric fields and crystal structure and lattice dynamics investigations based on a combination of Bragg and diffuse scattering data.

SNBL has two beamlines, BM01 and BM31, on the upgraded fourth generation EBS-ESRF storage ring. BM01 caters for Bragg diffraction and diffuse scattering, for single crystal, thin films and powder samples. BM31 is about to be upgraded and will be able to uniquely combine Bragg diffraction, X-ray absorption and high energy Total Scattering experiments on a single sample, both for powders and thin films. The available techniques provide in brief: high resolution and high intensity X-ray diffraction data on the average crystal structure at the atomic (Angstroms') scale. X-ray total and diffuse scattering data uncovering the local structure at the scale of few nanometers. Where XAFS relates to the average coordination and distance to neighboring atoms and XANES relates to the geometry and oxidation state by probing the electronic state.

In order the handle, the complex experiments all supported techniques are/or will be integrated in user-friendly control software together with auxiliary sample environment equipment, data visualization and on line analysis tools. This enables the staff and users to focus on their science and make optimal use of the beam time. Between 110 and 140 publications, appear every year with SNBL data. A team of seven scientists, technical, and secretarial staff support the user operation and continuous developments.
SNBL has two proposal deadlines per year: 1st March and 10th of September

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Email: thomas.weber@mat.ethz.ch

Website:
http://www.xray.mat.ethz.ch

Figure 1: The X-ray platform manager Thomas Weber

The X-ray platform of the Department of Materials at ETH Zurich offers a wide range of experimental possibilities in the field of X-ray diffraction, both for members of the department and for external users within and outside ETH. Among the available instruments are a kappa four-circle single crystal diffractometer, powder diffractometers in Debye-Scherrer and Bragg-Brentano geometry, a specialized instrument for thin film experiments and, expected to be available in autumn 2021, a small angle scattering diffractometer with a very wide range of additional equipment for measurements under non-ambient conditions. The platform covers typical materials science X-ray characterization methods, such as phase, texture, particle size, or crystallinity determination. In addition to teaching undergraduate and graduate students, joint PhD or post-doctoral projects are carried out if the scientific topic falls within the experience range of the platform manager. Specialty is local structure determination from diffuse scattering of disordered single crystals.

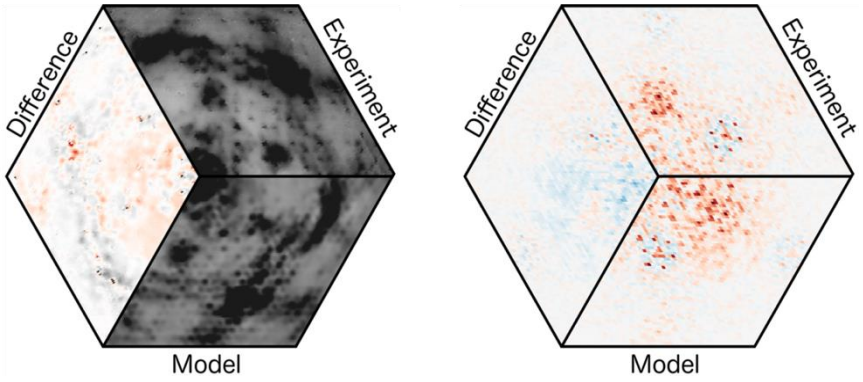

Figure 2: Sections of the diffuse scattering (left) and the three-dimensional difference pair distribution function, 3D-ΔPDF, (right), during a two-dimensional single-crystal-to-single-crystal polymerization at a conversion rate of 22% [1].

[1] Schlüter, A.D., Weber, Th., Hofer, G.: How to use X-ray diffraction to elucidate 2D polymerization in single crystals. *Chem. Soc. Rev*. (2020) **49**, 5140 – 5158.

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Figure 1: The Caflisch group as of December 2015. (Amedeo Caflisch is in the top left)

The Caflisch group (Figure 1) at Department of Biochemistry, University of Zurich, is interested in broad and multidisciplinary aspects of computational structural biology. To this end, we are developing new computational protocols for studying protein dynamics, in particular protein folding and disease-relevant protein aggregation, as well as new methodologies to investigate protein-ligand interactions in the context of structure-based drug discovery.
Our structure-based ligand discovery approaches make use of the structural information on protein-ligand recognition to serve as a starting point of further optimization. In our studies we screen *in silico* library of fragments, small and mainly rigid molecules that represent a large chemical space. We prioritize fragments by using proprietary *in silico* docking approaches (the SEED program [1]), validate their binding by using biophysical and biochemical methods, and confirm the predicted pose(s) by the means of protein X-ray crystallography (Figure 2). Fragments are then collaboratively developed to potent inhibitors by the means of structure- and *in silico*-guided medicinal chemistry. The group has identified a number of tyrosine kinase inhibitors with cellular potency, and a lead compound has shown excellent anti-tumor activity in a mouse model of breast cancer. More recently, we have developed small-molecule ligands for epigenetic reader proteins (human bromodomains [2]) and epitranscriptomic targets (the writer and readers of m6A-RNA [3,4]).

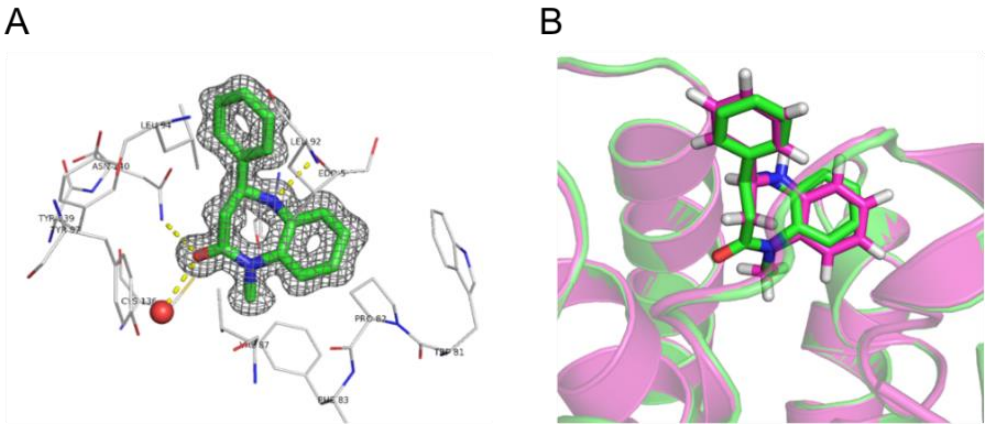


Figure 2: A) Crystal structure and experimental electron density of a fragment bound to the N-terminal bromodomain of the BRD4 protein (PDB code 4PCI). B) Comparison of docked (magenta) and crystal structure-derived (green) binding mode highlights accuracy of our computational docking methods.

The Caflisch group currently consists of nearly 20 people. Besides the development and application of computational methods for molecular dynamics and docking, and full in-house gene-to-structure capacity, the group includes also experts in cell biology, protein chemistry and biophysics.

[1] https://pubs.acs.org/doi/10.1021/acs.jcim.0c00556
[2] https://pubs.acs.org/doi/10.1021/acscentsci.7b00401
[3] https://pubs.acs.org/doi/10.1021/acschembio.9b00894
[4] https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/cmdc.202000011

Survey about the Swiss Society for Crystallography

(by Enrico Giannini)

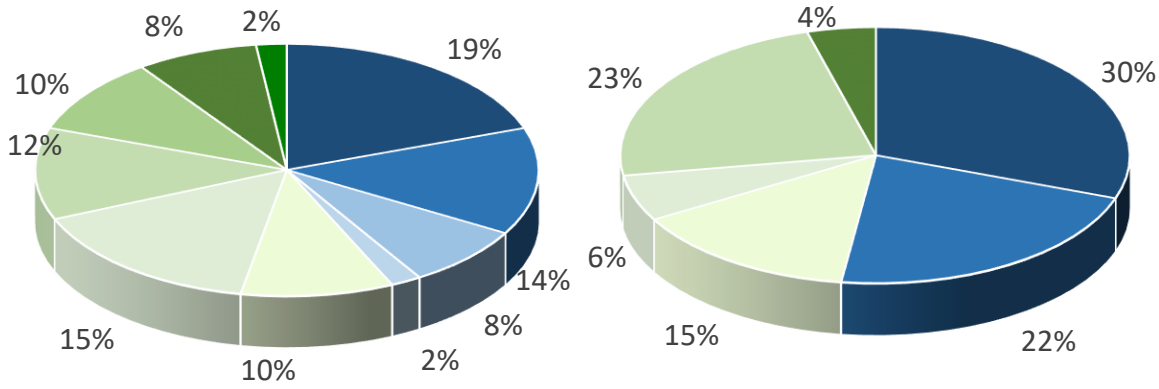
In July 2020 the members of the Swiss Society for Crystallography were invited to participate in a survey about the society, its missions and the interest the members find in it. About one third of the community has positively answered the invitation.

The members were interviewed about their background and profile, the type and availability of their laboratory facilities, their use of large facilities and their knowledge about the activities of the SSCr.

The scope of the survey was manifold: mapping the area of interest of the members, driving the SGK actions and policy in view of the Swiss roadmap for Photon Science, tuning and adapting the offer of the SSCr to the needs of the Community.

The segment of the community participating in the survey is likely to be largely composed of senior scientists, since with 22 out of 51 are “group leaders” (of any kind, professors or not) and 29 “non group leaders” (assistants, postdocs, retired members), and more than 50% are active either teaching crystallography, or educating students, or organizing schools (see Fig.1).

Fig. 1

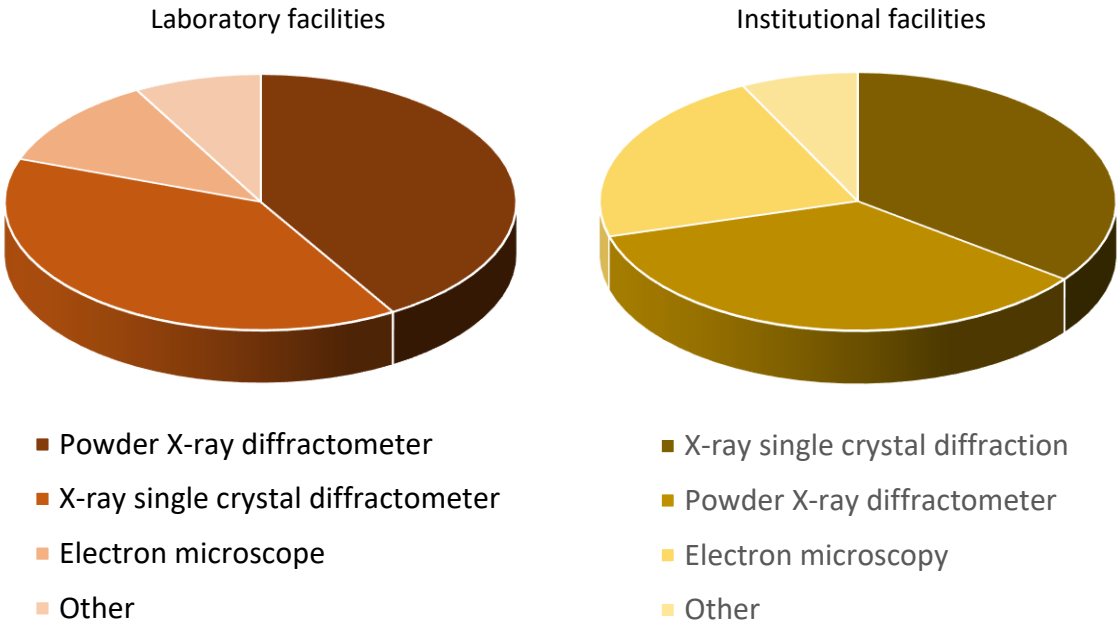


Career status:
Group leaders (prof. / no prof.)
Non group leaders (young scientists / students)

Education/Outreach:
Teaching / tutoring / school organisation
Doing only research

Most of laboratories are with equipped with either own or institutional diffraction facilities (see Fig.2). Half of them outsource the use of diffraction facilities.

Fig.2



More interesting, also in view of the future activity of the Swiss-Norwegian Beam-Line at ESRF, and the Swiss roadmap for Photon Science, is the information about the use of large-scale facilities. A majority of the participating members are regular users of large facilities (see Fig.3a). The Swiss facilities are the most used: various BL at the SLS, the SNBL at the ESRF, and the SINQ for neutron diffraction studies, cover together more than 50% of the total use of large facilities (Fig.3b).

Fig.3a
Use of large facilities

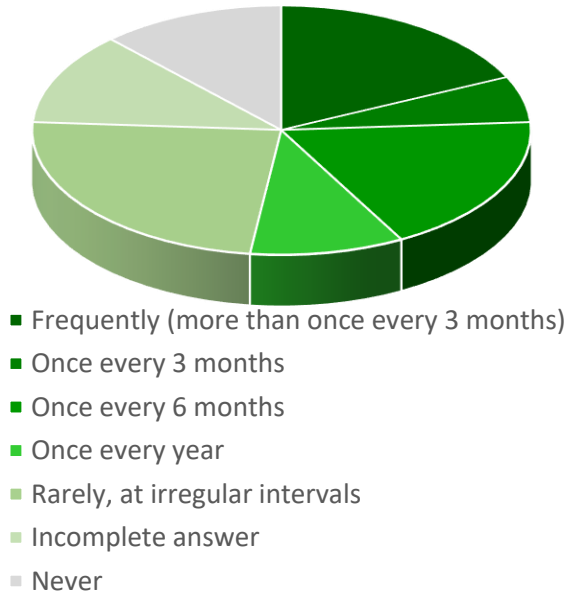
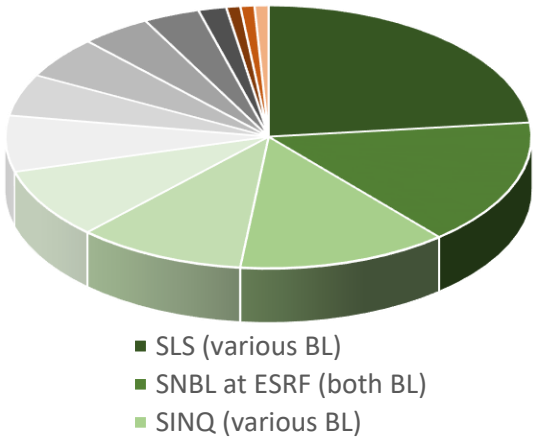


Fig. 3b

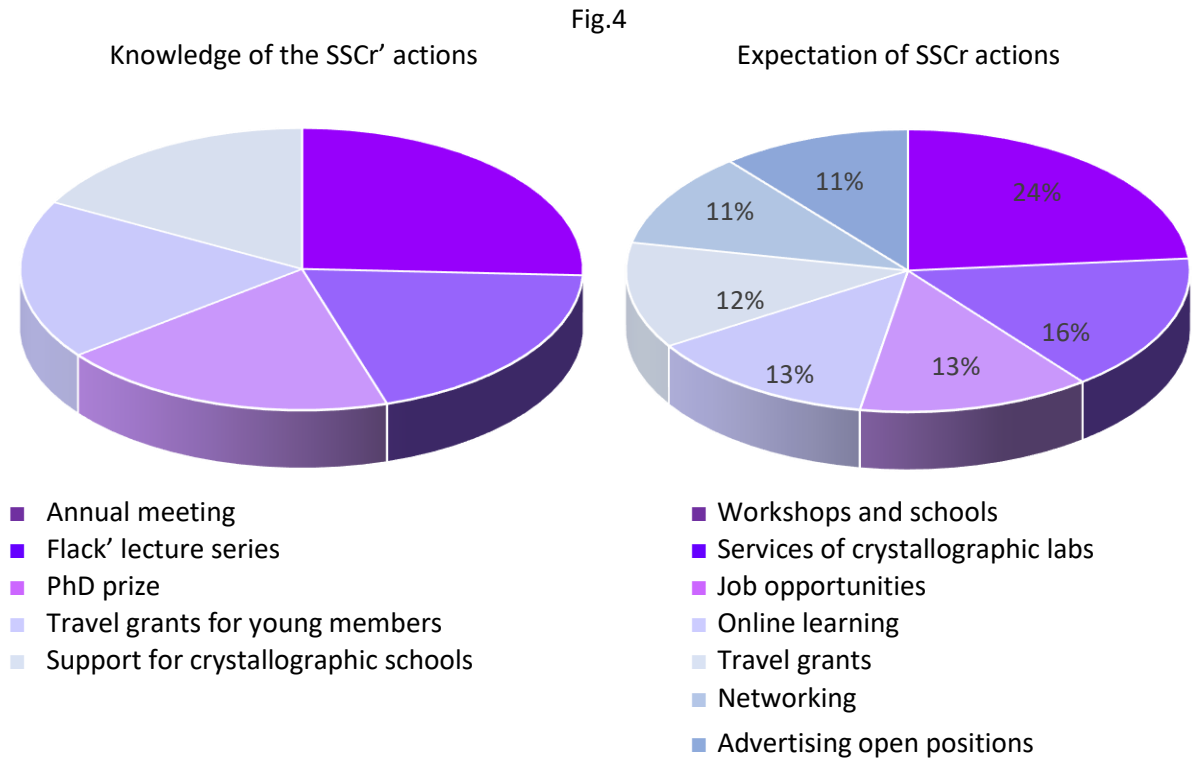


The users confirm the strong interest in using various beamlines at the international large facilities in the future, with a particularly increasing demand for the possibility to have beamtime at the Swiss beamlines at short notice and with simplified access procedures.

The majority of members of the SSCr are aware of the Swiss Roadmap for Photon Science, having been informed by the Society or personal contacts.

The last point of the survey is about the knowledge the members have of our society. As the following figure shows, the members of the SSCr know and appreciate all, and equally, the initiatives of the Society of the last years (left panel). Their expectations for future activities are also equally distributed, among crystallography-related workshops and schools, services of crystallography-related labs in Switzerland, job opportunities, online education initiatives, and networking (right panel). This encourages keeping the present course and going on with the initiatives launched in the last years.

Fig.4



Swiss Society for Crystallography PhD prize

The Swiss Society for Crystallography periodically offers a prize for the best PhD thesis in crystallography.

Requirements:

The prize is open to

a) Students, of any nationality, who earned a PhD title from a Swiss University
b) Students, of any nationality, who earned a PhD title from a University abroad, but carried out significant amount of work for the PhD title at a Swiss Research Institution, like EMPA, PSI or SNBL.
c) Students of Swiss nationality who earned a PhD title from any University worldwide.

The student must have earned the title between **March 31st 2019 and March 31st 2021**.

The subject of the thesis can be in any area of crystallography (structural biology, chemical crystallography, solid-state physics, crystallography of materials, etc.). The implications of the obtained results for crystallography should be evident.

Application:

The application for the prize should be submitted before **31st May 2021** by the student himself or by the thesis supervisor. The applicant should submit: a) a pdf copy of the thesis; b) a letter of the supervisor approving his/her candidature; c) pdf copies of the articles published from the results obtained during the thesis; d) a pdf scan of the PhD diploma; e) a short CV of the candidate. Applications for this SGK Thesis Prize are accepted only once per applicant.

The application should be sent to the secretary of the Swiss Society of Crystallography (info@sgk-sscr.ch)

The award

The winner will be selected by a commission, based on the quality of the research, the quality of the publications, and the effective contribution of the candidate to the scientific work. The commission may decide not to assign the prize if none of the candidates fit the minimal prerequisites concerning the topic, the quality of the thesis, the papers published from it and the approval of the supervisor.

The winner will be announced before the annual meeting and will be invited to give a short talk of the results of his/her thesis.

The Swiss Society of Crystallography will award the winner with a diploma and will reimburse the participation of the student to the annual meeting.

The award is endowed with 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 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

Due to the limited meeting and travel possibilities this year, the remaining funds from 2020 will be available additionally for 2021. Nonetheless, if you are attending a meeting later this year, or have recently attended a 2020 meeting, you are welcome still to apply for 2020 support.

New Board Members

The SGK/SSCr is looking for two new board members starting Sept 2021. Interested members may apply, please include one support letter of a member.

Meetings, Conferences, Workshops, Schools, Courses

More info at: https://www.xray.cz/iucr/

The Zürich School of Crystallography

More info at: https://www.chem.uzh.ch/linden/zsc/

IUCr XXVI

26th Congress & General Assembly of the International Union of Crystallography 2023
22 Aug 2023–29 Aug 2023 in Melbourne, Australia
More info at: https://scanz.iucr.org/

7th European Conference on Crystal Growth, ECCG7

Date: July 25-27, 2022
Venue: Marriott Rive Gauche Conference Center, Paris, France
https://www.escg3-eccg7-paris2021.insight-outside.fr/

3rd European School on Crystal Growth, ESCG-3

Date: July 20-23, 2022
Venue: Chimie-Paris (IRCP) and Physico-Chemical Biology Institute (IBPC), Paris, France
https://www.escg3-eccg7-paris2021.insight-outside.fr/

EPDIC17

https://www.epdic17.org/

Positions

Wissenschaftliche/r Mitarbeiter/in für die wissenschaftliche Betreuung der Einkristallröntgenstrukturananlyse an der Universität Jena:
Weitere Informationen:
https://www4.uni-jena.de/Universit%C3%A4t/Stellenmarkt/Wissenschaftliche+Besch%C3%A4ftigte/Wissenschaftlicher+Mitarbeiter+%28m_w_d%29-p-597001.html

Calls for proposals

Beside normal proposals, most facilities allow urgent beam time requests. Please check directly with the facility.

Facility	Deadline(s)	Link
Priority access call for work on combating COVID-19, see		www.psi.ch/useroffice/
For news about current situation SLS, SwissFEL, see		www.psi.ch/useroffice/
SLS: Swiss Light Source		
All except PX lines	15.03. and 15.09.	https://www.psi.ch/de/useroffice/proposal-deadlines
Protein crystallography beamlines (PX)	15.04. and 15.10.	
SINQ: Swiss Spallation Neutron Source		
All instruments (regular calls)	Nov. 15, May 15	https://www.psi.ch/de/useroffice/proposal-deadlines
SINQ/SLS		
Joint x+n proposals (MS/HRPT)	26.02.	https://www.psi.ch/de/useroffice/proposal-deadlines
SμS: Swiss Muon Source		
DOLLY, GPD, GPS, HAL-9500, LEM	Dec. 9,	https://www.psi.ch/de/useroffice/proposal-deadlines
SwissFEL		
ARAMIS-Alvra, ARAMIS-Bernina	15.03, 15.09	
ESRF: European Synchrotron		
long term proposals	15.01.2021	www.esrf.eu/UsersAndScience/
short term proposals (standard)	01.03.2021	
ILL: Institut Laue Langevin		
All instruments	15. 02. 2021	www.ill.eu/
FRM II: Heinz Maier-Leibnitz		
All instruments	tba	www.mlz-garching.de/user-office/
Rapid access program	tba	www.mlz-garching.de/user-office/
SNS Spallation Neutron Source	24.03.2021	neutrons.ornl.gov
Oak Ridge		

Calendar of forthcoming meetings

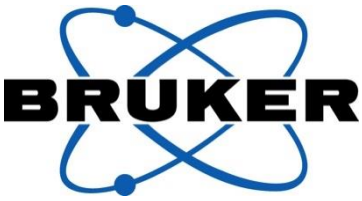
(Please mail the missing information on meetings of interest to woerle@inorg.chem.ethz.ch)

News from the IUCR about the **Melbourne Congress and General Assembly of the IUCr**
https://www.iucr.org/news/notices/announcements/26th-iucr-congress#.XqYdlcJJGvU.twitter

			Application Deadline
2021			
Aug. 14-22	Prague, CZ	25th Congress & General Assembly of the IUCR, Congress postponed to August 2021 https://www.xray.cz/iucr/	Abstracts for Lectures: 15.04.2021
2022			
May 31-June 3	Šibenik, HR	EPDIC17, https://www.epdic17.org/	01.03.2022
June 19-30	University of Zurich	Zurich School of Crystallography http://www.chem.uzh.ch/linden/zsc	tba
July 20-23	Paris, F	3rd European School on Crystal Growth, ESCG-3 https://www.escg3-eccg7-paris2021.insight-outside.fr/	tba
July 25-27	Paris, F	7th European Conference on Crystal Growth, ECCG7 https://www.escg3-eccg7-paris2021.insight-outside.fr/	Abstracts: 16.05.2022
Aug. 23-27	Versailles, F	33rd European Crystallographic Meeting https://ecanews.org/	To be announced
2023			
Aug. 22-29	Melbourne, Au	26th Congress & General Assembly of the IUCR, https://scanz.iucr.org/	To be announced

Institutional members and supporting institutions

Corporate members



Supporting institutions

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

Become a member of SGK/SSCr

If you are working in the field of crystallography, you might be interested in becoming a member of our society. For more information as well as online registration, please go to our website (http://www.sgk-sscr.ch).
Presently, the yearly membership fee is CHF 40 (CHF 10 for students).

SGK/SSCr is a member of the Swiss Academy of Science.

Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

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