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

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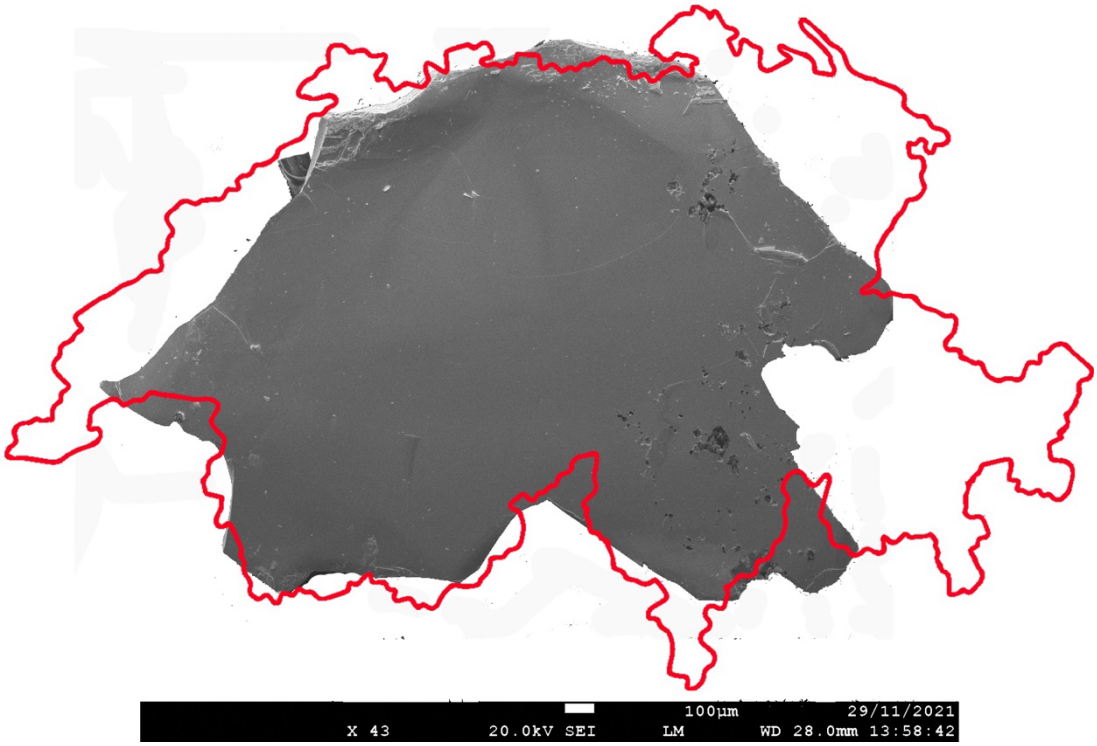


In this issue: The Howard Flack Crystallographic Lecture Series: electron crystallography
Announcement Annual Meeting and General Assembly 2022 in Bern

On the cover:
Switzerland-shaped crystal of Pt2HgSe2, a novel topological material offering an exciting Quantum Spin-Hall insulating behaviour (UniGe and EPFL), grown in the Laboratory for Quantum Materials Discovery, DQMP, University of Geneva.
Ref: Cucchi et al., Physical Review Letter 124, 106402 (2020)

The President's Page

Dear Members of the Swiss Society for Crystallography,

this is my first message to you as president of the society. A little surprised given my comparatively young age, I was elected president of the Swiss Society for Crystallography at the general assembly during our annual meeting in Bern, 2022. I consider it an honour that the society entrusts me with this assignment and, while surely a challenge, I am motivated and looking forward to represent our society throughout the next three years. I would like to thank Simon Grabowsky for joining in as vice-president and also to welcome Paula Abdala (ETHZ) as our newest board member. In particular, my warm thanks go out to Antonia Neels, who has given us direction and guidance during the last three years.

I joined the society in 2010 upon arriving in Switzerland, at the time to join the Laboratory of Crystallography in Geneva for my doctorate. Twelve years later I have got to know and appreciate many colleagues in Switzerland, visited their institutes and labs, participated in heaps of interesting projects and done countless experiments, developing quite a passion for structural sciences and the involved technicalities in all aspects. I consider modern crystallography an extensive powerful toolset that allows us to become creative in so many fields of science. In line with this, I work at the interface between a user facility and interdisciplinary science at the Institute of Chemistry and Chemical Engineering of EPFL.

Together with a partially reformed board whom I look forward to working with, I would like re-visit our outreach to our members and colleagues, and the ways we disseminate crystallographic content and education. We have already started with a new webpage reached by a new user-friendly domain name swiss-crystallography.ch, and you can now follow us on twitter as well: @Swisscrystallog. During our annual meeting, which will be hosted by Simon Grabowsky in Bern, September 15th, we suggest to have a round-table-discussion on future topical SSCr workshops, which the board would like to organize on an annual basis starting in 2023. In order to plan this we need in particularly student feedback and strongly encourage graduate and undergraduate students to attend the session reserved for this. You are the target group and we want to design such workshops according to your needs!

2022 will be a busy year throughout which we will catch up on things that were on stand-by during the pandemic. Our Howard Flack Crystallographic Lecture Series is going to be personal again and we are grateful to have Lukáš Palatinus from the Czech Academy of Sciences as our Flack Lecturer, who will visit Switzerland on a six-stop tour in November 7th – 11th, speaking to us on the exciting and timely topic of Electron Crystallography.

Though life is nearly back to normal in Switzerland, it is very different elsewhere and not only many colleagues and friends are struggling to ensure their livelihood. In this context the board has announced a scholarship in support of Ukrainian students, which was first awarded beginning of April to a first excellent candidate, and with a second call taking place very soon.

Finally, let me invite and encourage you to contribute to our newsletter, as well as to our digital channels. Just drop us a message with a little write up on your research highlights, your favourite experiments or just everyday lab-life.

All the best for 2022!

Pascal Schouwink

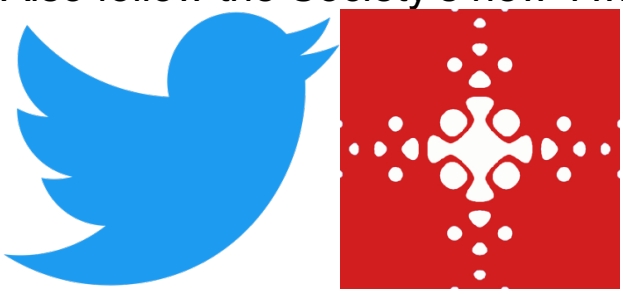
President of the SGK-SSCr

SGK-SSCr new website and Twitter account

Deplorably, the Society's old web domain sgk-sscr.ch has been hijacked. The Society decided to refuse to pay ransom for the old domain name and opted for a fresh start. Members and crystallographers in Switzerland and elsewhere from now on will found our published content on

https://swiss-crystallography.ch

Also follow the Society's new Twitter account



Swiss-crystallography
@Swisscrystallog

Obituary

Jack David Dunitz and chemical crystallography (1923-2021)

Jack Dunitz, emeritus professor of chemical crystallography at the laboratory of organic chemistry of the Eidgenössische Technische Hochschule Zürich (ETHZ), passed away on September 12, 2021, at the age of 98 years. Jack was a leading figure in chemical crystallography. He addressed and solved a broad range of chemical problems with the help of structural information from diffraction experiments. Jack himself reviewed his early life in science in an essay entitled 'La Primavera'[1]. In several conversations he reflects on his time at ETHZ.[2,3]

Jack was born in 1923 in Glasgow. For his Ph.D. he worked with J. Monteath Robertson on structures with H, C and O atoms only (long before direct methods). During his wanderings through labs in Oxford, Pasadena, Bethesda and London he learned from the best: Dorothy Hodgkin, Linus Pauling and Sir Lawrence Bragg among others. During his early carrier he published and joined ranks with the group of people who would constitute the core of chemical crystallographers in the second half of the 20th century, among them Leslie Orgel (ferrocene) and Verner Schomaker (cyclobutane).

In 1957 Jack became professor of chemical crystallography at ETHZ where he stayed active until long after his retirement in 1990. Initially Jack determined structures of saturated, medium-sized carbon and lactam ring compounds. These studies were a rich source of information on strained bond and torsion angles, answered tantalizing questions concerning unexpected trans-annular chemical reactivity and preferred arrangements of substituents.

With the advent of diffractometers and main frame computers it became possible to investigate families of related compounds in a reasonable amount of time and to correlate aspects of their structures. Jack's best known 'structure correlation' shows a nucleophilic nitrogen atom approaching an electrophilic carbonyl carbon atom with an N…C=O angle of ~105° (Bürgi-Dunitz angle). Up to the mid-nineties most meetings on crystallography featured lectures or microsymposia on 'Structure Correlation'.

Jack pursued many other scientific interests reviewed in his book 'X-ray Analysis and the Structure of Organic Molecules':[4] ion-selectivity of ionophores, hydrogen bonds to organic fluorine, atomic and molecular motion, first order phase transitions. For Jack, the crystallographer, symmetry was a *sine qua non* as it was for his chemistry friend

E. Heilbronner. Together they wrote '*Reflections on Symmetry in Chemistry… and elsewhere'*.[5]

Jack liked problems, puzzles and mysteries, e.g. the missing bonding electrons in C-F bonds or the disappearing polymorphs. He didn't always find the ultimate answer to open questions, but his essays on everything he wrote about are erudite, profound, interesting and entertaining. Clear language was important to Jack. His attitude lives on in Dunitz' rule: 'Almost every scientific paper can be improved by deleting the first sentence.'

Jack's work was widely recognized: He was an Honorary Member of the Swiss Society for Crystallography, the Swiss Chemical Society, the British Crystallographic Association

and the Royal Society of Chemistry. He was awarded the centenary Prize of the Royal Society of Chemistry (1977, with G. Olah and K. S. Pitzer), the Paracelsus Prize of the Swiss Chemical Society (1986), the Gregori Aminoff Prize of the Royal Swedish Academy of Sciences (1990), the Buerger Award of the American Crystallographic Association (1991), the Havinga (1980) and Bijvoet medals (1989). Jack was elected Fellow of the Royal Society of London and member of the German Academy of Sciences Leopoldina, the Academia Europaea and the European Academy of Sciences and Arts; he was a foreign member of the Royal Netherlands Academy of Sciences, the U.S. National Academy of Sciences, the American Philosophical Society, and the American Academy of Arts and Sciences. Jack was awarded honorary doctorates from the Technion (1990), the Weizmann Institute of Science (1992) and the University of Glasgow (1999).

Jack expressed his stance towards crystallography in a short essay on the future of crystallography : '… if crystallography has an uncertain future it has a great past and it still possesses the rare intellectual charm of relating to the three basic sciences, physics, chemistry and mathematics, as well as to the decorative arts. It should not be taught or studied in a too restrictive, introspective manner' (Dunitz, 2002).[6] Jack's writings express this 'rare intellectual charm' and he and his work certainly are an integral part of crystallography's 'great past'.[7]

[1] Dunitz, J.D. (2013) *Helv. Chim. Acta*, **96**, 545-563

[2] Two-part video interview with Jack by Erik Carreira, ETHZ (2021) https://www.youtube.com/watch?v=bCTMoUEH5ts&list=PLjdmj19Qw3bp9idjAh6Ucvyhf1XUKflP5&index=10; https://www.youtube.com/watch?v=jN03OQLfjrI&list=PLjdmj19Qw3bp9idjAh6Ucvyhf1XUKflP5&index=11

[3] Carafoli, E., Dunitz, J.D. (2017) *Biochem. Biophys. Res. Commun.*, **492**, 1-17; Weber, L., Dunitz, J.D. (2011) *Chimia*, **65**, 440-443

[4] Dunitz, J.D. (1979*) X-ray Analysis and the Structure of Organic Molecules*, Cornell University Press; Dunitz, J.D.(1995) *X-ray Analysis and the Structure of Organic Molecules* (corrected reprint), Verlag Helvetica Chimica Acta.

[5] **Heilbronner, E., Dunitz, J. D. (1993)** *Reflections on Symmetry in Chemistry … and Elsewhere.* Verlag: Weinheim. VCH Verlagsgesellschaft.

[6] Dunitz, J.D. (2002) *Zeitschrift für Kristallographie - Crystalline Materials*, **217**, 299-300.

[7] This text is an adaption of a more detailed obituary: Bürgi, H.B. (2022) *Acta Cryst B*, **78**, doi.org/10.1107/S2052520622001366

Picture by Jay Siegel

Howard Flack Crystallographic Lecture Series

Swiss Society for Crystallography

The Howard Flack Crystallographic Lectures Series

On the Topic:

'Electron Crystallography'

This year's Howard Flack Lecture Series will focus on electron crystallography, with **Lukáš Palatinus** as our invited Flack Lecturer. A crystallographer by education, Lukáš has for a long time been driving developments regarding crystallographic software and diffraction methods, with a particular focus on electron diffraction. Events will be held on-site.
Details soon on:
swiss-crystallography.ch/en/flack_lectures and twitter.com/Swisscrystallog

7th – 11th November 2022
ETHZ, 07.11 – PSI, 07.11 – Uni Basel, 08.11 – Uni Bern, 09.11 – EPFL, 10.11 – Uni Geneva, 11.11

Dr. Lukáš Palatinus, FZU, Czech Academy of Sciences

Lukas Palatinus studied mineralogy and geochemistry at the Charles University in Prague. During his PhD. at the University Bayreuth, Germany, he focused on the crystallographic analysis of modulated structures. Later, during his post-doctoral stay at the EPFL, Lausanne, Switzerland, he developed the program Superflip for the solution of the crystallographic phase problem for periodic and aperiodic crystals, using the iterative dual space algorithms.
Since 2009, Dr. Palatinus is the head of the group of electron crystallography at the Institute of Physics of the Czech Academy of Sciences in Prague. He and his co-workers are developing methods for crystal structure analysis from electron diffraction data, with the main focus on the structure refinement from 3D electron diffraction tomography data using the dynamical diffraction theory.

The lectures will be focused on the theory and practice of 3D electron diffraction (3D ED) – a crystallographic technique allowing structure analysis from single submicrometric crystals. This technique was born almost two decades ago, but it is now going through a phase of explosive development. Some eight years ago its general applicability and achievable accuracy was still a matter of debates. Five years ago, first reports showing reliable localization of hydrogen atoms by 3D ED appeared, and refinements with figures of merit approaching those of X-ray diffraction became possible. Today, observation of hydrogens and other structural details is considered routine, and advanced applications like charge density analysis from 3D ED data are appearing.

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.

2022 SGK-SSCr Meeting Announcement

Swiss Crystallographic Association,
Annual Meeting 2022

Date: September 15th (all day), and September 14th (Conference Dinner)
Place: Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Freiestrasse 3, 3012 Bern.
Format: On-site only, no virtual or hybrid options.
Website: http://www.dcbp.unibe.ch/sgk2022
Registration: Registration and abstract submission is open. Registration is free of charge. For participation at the conference dinner at Altes Tramdepot (https://www.altestramdepot.ch/), a contribution of CHF 65 is required that can be paid during registration.
Invited Speakers:

Enrico Mugnaioli (University of Pisa) in the session "Materials and Minerals"

Andreas Engel (Biozentrum Basel) in the session "Structural Biology"

Simon Parsons (University of Edinburgh) in the session "Chemical Crystallography"

See you soon in Bern!

2022 SGK-SSCr Meeting Programme

Scientific Programme

Annual Meeting Swiss Society for Crystallography

15 September 2022

UNIVERSITÄT BERN

08:30		Registration & coffee
09:20	Simon Grabowsky	Welcome address
09:30 – 10:30	Chairs: Sergey Churakov, Georgia Cametti	**Materials and minerals**
9:30 – 10:00	Speaker: Enrico Mugnaioli	Title tba
10:00 – 10:15	Tba	Talk from abstracts
10:15 – 10:30	Tba	Talk from abstracts
10:30 – 11:00		Coffee break, **posters** and sponsors
	Chair: Paula Abdala	**Large user facilities in Switzerland**
11:00 – 11:12	Nicola Casati	Swiss Light Source
11:12 – 11:24	Dmitry Chernyshov	Swiss Norwegian Beamlines, ESRF
11:24 – 11:36	Céline Besnard	Dubochet Center for Imaging
11:36 – 11:48	Bill Pedrini	SwissFEL
11:48 – 12:00	Romain Sibille	Laboratory for Neutron Scattering and Imaging
12:00 – 12:30	Chair: Pascal Schouwink	**Round table discussion on future SSCr workshops**
12:30-14:30		Lunch, **posters** and sponsors
13:30-14:30	for SSCr members	**SSCr annual general assembly**
14:30 – 15:30	Chair: Achim Stocker	**Structural biology**
14:30 – 15:00	Speaker: Andreas Engel	Cryo electron microscopy of crystals and single particles
15:00 – 15:15	Tba	Talk from abstracts
15:15 – 15:30	Tba	Talk from abstracts
15:30 – 16:00		Coffee break, **posters** and sponsors
16:00 – 17:00	Chairs: Hans-Beat Bürgi, Lorraine Malaspina	**Chemical crystallography**
16:00 – 16:30	Speaker: Simon Parsons	Title tba
16:30 – 16:45	Tba	Talk from abstracts
16:45 – 17:00	Tba	Talk from abstracts
17:00		**Poster prize** and farewell apéro

Report SGK/SSCr Annual Meeting 2021

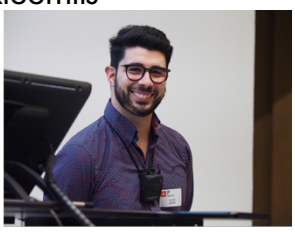
After a report of the Annual Meeting 2020, the 2021 session was held at the University of Fribourg in a live version. It was a good opportunity to meet in real our colleagues and members of the society. Like in the past years, the general organization was covering the full day with a scientific program and a general assembly after lunch time. The meeting was articulated over the “theme”: “From molecules to nanoparticles in biology, chemistry, physics and geology”. The day was divided over three main orientations: Chemistry, Materials and Biology each session was open with presentation of Prof. Catherine Housecroft, “*The terpyridine isomer game: ditopic and tetratopic ligands with 4,2':6',4''- and 3,2':6',3''-terpyridine metalbinding domains in metal-organic networks*”, Prof. Nicola Hüsing, “*Hierarchically Organized Porous Metal Oxides, Carbons and Hybrids: Non-Conventional Sol-Gel Precursors and Processes”* and Prof. Robin Teufel, “*O_2-pressurized X-ray crystallography as Tool to Study Flavoprotein Oxygenases in Natural Product Biosynthesis”.* It was also the occasion to reward Florian Kleemiß for his Crystallography PhD Prize 2021, "*Development of quantum-crystallographic methods for chemical and biological applications*".
The poster prize was attributed to Margarita Rekhtina for her poster: “*MgO-based CO_2 sorbents: formation of $MgCO_3$ at buried $NaNO_3$-MgO interface investigatied by X-ray grazing incidence diffraction, reflectometry, and electron microscopy”.*
Thanks to all particiapants for this day.


Catherine Housecroft


Nicola Hüsing

Robin Teufel

Florian Kleemiß



2021 Howard Flack lectures: report

2021 Howard Flack Lecture Series

After only two installations of the Howard Flack Lecture Series in 2018 and 2019, it had to be suspended in 2020 because of the Covid outbreak. For 2021, returning to the original mode of a lecture tour of an invited speaker through Switzerland seemed unrealistic. Therefore, we decided to reverse the scheme and instead of one person visiting many Swiss labs, we asked many Swiss labs to present themselves to a national (and international) crystallographic audience using an online platform provided by the EMPA Academy. All lectures came from the field of **structural biology** as this is a rapidly developing field that incorporates many new and exciting techniques and methods, most of which are directly related to crystallography.

The opening lecture was given on February 18th by **Andrea Thorn** (University of Hamburg) on the Coronavirus Structural Taskforce.

The first talk by one of the Swiss structural biology groups was given by **Gebhard Schertler** (ETH Zürich and PSI) on March 15th. He talked about SwissFEL adventures in room-temperature crystallography for optogenetics and to elucidate rhodopsin structures (Figure 1, top).

On April 12th, **Stefan Salentinig** (University of Fribourg) talked about bioinspired materials for functional foods.

A lecture by **Dimitrios Fotiadis** (University of Bern) concluded the spring semester on May 18th. He explained the role of water molecules and networks in ligand binding.

In the autumn semester (September 13th), **Michael Hothorn** (University of Geneva) restarted the lecture series with a discussion of plant signal transduction cascades.

Jan Pieter Abrahams (University of Basel) talked about the catalytic cycling of the human mitochondrial Lon protease homolog using studies by cryo-EM techniques on October 11th.

The final lecture was delivered by **Amedeo Caflisch** (University of Zurich) on November 15th about protein structure-based drug design involving theoretical methods (Figure 1, bottom).

With this lecture series, our Society experimented for the first time with a fully online presentation mode. Moreover, we tried to build a link between the structural biology field and the, in the past, more materials- and small-molecule oriented member base of the Society. With fluctuating participation numbers of between 40 and 150 as well as stimulating discussion sessions, the 2021 Howard Flack Lecture Series was a great success. The Society will continue to more strongly involve both researchers from the structural biology field and electronic possibilities of reaching out in their future Annual Meetings and Howard Flack Series.

Simon Grabowsky

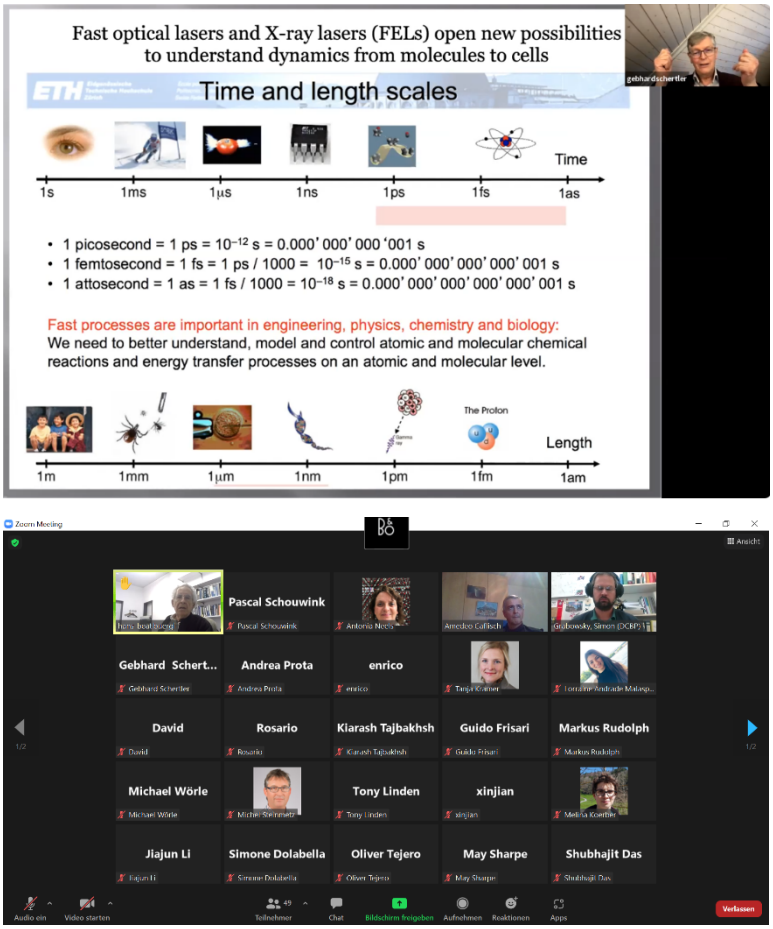


Figure 1. Top: Gebhard Schertler's lecture on opportunities of X-ray free electron lasers.

Bottom: Hans-Beat Bürgi asking questions to Amedeo Caflisch after his lecture.

Report on the Workshop for the Swiss Norwegian Beamlines (SNBL) 2022

SNBL workshop 2022, April 5th, Bern. Organizing committee: Wendy Queen (Chair), Radovan Černý, Paula Abdala, Simon Grabowsky, and the Swiss Steering Committee (SSC) of the SNBL.

The SNBL Workshop 2022 was held on April 5th at the University of Bern. The event took place in a convivial atmosphere, in a hybrid mode (i.e., including both on-site and on-line options) and with ca. 70 registered participants. Most of the participants were on-site, but also some of them, who were unable to travel for various reasons, joined on-line. The goals of the Workshop were focused on connecting SNBL users and beamline scientists, attracting new users and providing insight into the many ways SNBL can serve our Swiss scientific community in material's characterization. With a rich program and a high level of presentations and discussions, the workshop was successfully realized.

Radovan Černý opening the Workshop.

Prof. Radovan Černý (UniGe) opened the event with a welcoming speech, which was followed by an update on the EPFL/ETHZ takeover of SNBL and the most recent upgrade by Prof. Wendy Queen and Dr. Paula Abdala. The program included two excellent plenary lectures by invited international speakers: "Studying correlated disorder with X-rays" by Prof. Andrew Goodwin (Oxford University) and "Advances in the operando X-ray analysis of heterogeneous catalysts" by Prof. Bert Weckhuysen (Utrecht University). Two very active sessions (Charis: Profs. Simon Grabowsky and Prof. Raffaella Buonsanti) hosted elevator pitches from various groups in Switzerland, on research and related pressing questions that SNBL might help answer. The speakers of these sessions were: Prof. Maksym Yarema (ETHZ), Prof. Jovana Milic (UniFribourg), Prof. Thomas Buergi (UniGe), Prof. Takuji Adachi (UniGe), Till Schertenleib (EPFL), Dr. Sharon Mitchell (ETHZ), Prof. Murielle F. Delley (UniBasel), Dr. Seongmin Jin (EPFL), Prof. Peter Broekmann (UniBern) Prof.

Jonathan De Roo (UniBasel), Prof. Raffaella Buonsanti (EPFL) and Dr. Simonov Arkadiy (ETHZ). The topics presented included research on a wide variety of advanced and functional materials, with focus on their in-depth structural characterization. Especially these presentations discussed: hybrid perovskite materials for renewable energy conversion, fundamental insight into the synthesis of nanocrystals with controlled phase and composition, understanding structure-performance relationships in heterogeneous catalysts for sustainable applications, development of well-defined metal-organic frameworks for applications such as CO_2 sorption and in catalytic process, as well as the fundamentals of materials with correlated disorder. Highlights of the applications of BM01 and BM31 stations of SNBL for materials characterization were presented by Dr. Dmitry Chernyshov (Senior Beamline Scientist BM01), Dr. Dragos Stoian (Beamline Scientist MB31) and Dr. Wouter Van Beek (SNBL director). Emphasis was given on advanced in situ/operando capabilities, new computational tools for big data analysis, and novel opportunities for combined techniques created in these facilities.

The meeting successfully gathered the Swiss scientific community around the quest for advanced materials characterization techniques. The Swiss Crystallography Association took an active role in the meeting by participating in various discussions and providing an updated on the latest news of SSCr by Dr. Dubravka Sisak Jung.

Members of the SSCr board participating in the Workshop.

The closing session of the workshop was chaired by Prof. Wendy Queen who motivated interesting debates. Most participants engaged in the discussions, and it quickly became clear that SNBL is a very valuable tool for the Swiss materials science, chemistry, catalysis, and the crystallographic community in general. The unique energy range and combination of techniques was emphasized as well as the complementarity with the facilities at the Swiss light source (SLS). In this context, SNBL could likely play an active role during the dark period of the planned SLS-II upgrade.

However, it was also evidenced that access costs are in many cases difficult to face for various research groups. It is worth mentioning that SNBL has gone through an institutional and financial transition in recent years. Since 2020, SNBL is managed by the EPFL and is available to Swiss users on a pay-per-use model. Currently, different universities, namely EPFL, UniGe, and ETHZ, fund 2/3 of the costs of beamtime for their users, alleviating the cost of access for the research groups. However, this is not the case for many universities and other research facilities in Switzerland that must pay the full price of the shift. The price of beamtime access is for many research groups not affordable and, thus it was seen as a problem. The debate on how to guarantee access to these indispensable facilities for Swiss users to maintain their high level of scientific research in the coming years and beyond 2024 is still open.

In terms of beamtime access mode, some of the participants expressed that their research could benefit from a fast access (e.g., within 3 months between proposal and experiment being performed) and long-term (2-years) projects.

Lastly, one topic that received a lot of attention was the need of specialized schools for new users (especially PhD students, postdocs) particularly for the analysis of big

data. The SNBL Swiss board, the SSC of SNBL, and the SSCr would be involved in organizing such events.

Paula Abdala – Wendy Queen – Radovan Černý

SGK-SSCr Scholarship for students from Ukraine

The SGK-SSCr launched a scholarship for Ukrainian students in Switzerland that find themselves in dire economic straits due to the war. It is meant to provide sustain to the affected student(s) through a short bridging period while more permanent solutions are pursued.

The first call (deadline 27.03.2020) has been successful. Of the applicants, Ms. Oksana Shlyahtun (M.Sc.) has been found eligible and has been awarded the sum of CHF 6300 (after taxes) to support her living costs for 2 months. After that, she will start with a PhD position in the group of Prof. Davide Bleiner, EMPA Dübendorf.

An interview to Oksana on the Swiss public TV SRF can be listened to at the link

https://www.srf.ch/audio/rendez-vous/ukrainische-wissenschaftler-innen-in-der-schweiz?partId=12174435

After the successful first call, a new call is being presently launched, whose deadline will be at the end of June 2022.

Implementing 3D- electron diffraction in the Dubochet Center for Imaging Geneva.

Maxime Patigniez, Mohamed Salamoun, Yashar Sadian and Céline Besnard.

During the last years, 3D-ED has been attracting attention as a potential new tool for structure elucidation. The strong interaction between the electrons and the sample allows to collect data from small crystals, of the order of tens to hundreds of nanometres in size. As a result, this method has raised a strong interest among scientist in need of structural information (Gemmi *et al.*, 2019). Figure 1 shows the same organic powder sample measured on a conventional home-lab x-ray diffractometer, where a typical powder diffraction pattern is obtained and in a Transmission Electron Microscope, where the diffraction pattern from a single small crystal can be recorded. Being able to obtain single-crystal data from such samples appeared of great interest to us so we decided to implement 3D-electron diffraction in the university of Geneva.

The Dubochet Center for Imaging (DCI) is a joint initiative of the EPFL, the University of Lausanne and the University of Geneva. The DCI is attended as a service platform for cryo-electron microscopy and is currently composed of two sites, one in Lausanne and one in Geneva. We equipped one of the Transmission Electron Microscopes of the DCI Geneva (200 kV FEI Tecnai G2 Sphera) with a retractable hybrid pixel detector from Amsterdam Scientific (Figure 2). With such a fast detector, it is quite straightforward to collect 3D diffraction data by tilting the sample holder of the transmission electron microscope while recording a series of frames. This is similar to a phi scan for conventional X-ray data and once the rotation axis is identified, conventional programs for x-ray data or dedicated electron diffraction data software can be used to process the data. We have been using Cred(Wan *et al.*, 2013), PETS(Palatinus *et al.*, 2019), DIALS(Clabbers *et al.*, 2018) and CrysAlis PRO(Rigaku Oxford Diffraction, 2022) to examine and process the data.

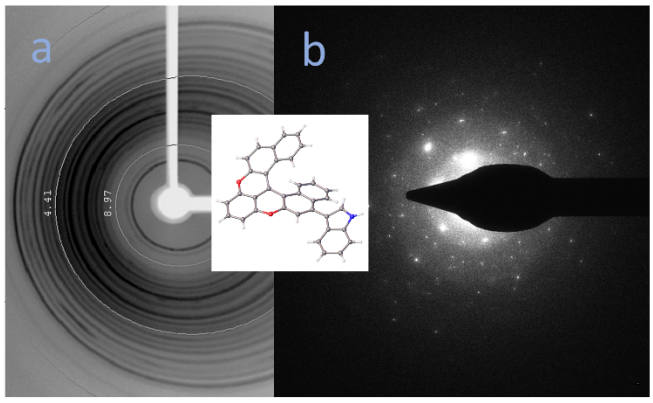


Figure 1. The same organic sample measured a) with a Rigaku Smartlab putting the sample in a loop and using X-ray radiation and b) with electron diffraction using the tecnai G2 sphera at 120KV (CCD camera eagle). Using electron diffraction, we can measure diffraction from a single grain.

Our setup allows us to record datasets in a few minutes for crystals of a few hundreds of nanometres. If the sample is a dry powder, the preparation is relatively easy. The grid is travelled into the finely ground powder and the excess powder is removed by gently tapping the grid. A few trials may be necessary to get a good grid, in which single grains can be isolated. Once the grid is obtained, a few hours may be necessary to collect sufficient good datasets that will be merged to increase the completeness and hence the chances of a straightforward data solution.

The data quality is at first hand very disturbing for a “conventional” x-ray crystallographer. The Rint can be unusually high, the scaling of the data can be problematic. The selection of the best datasets and the rejection of bad parts in the

measured dataset (the crystal may move slightly out of the beam during the data collection for example) is not a straightforward process at first.
Structure solution using Superflip, SHELXT or SHELXD goes relatively well, once a decent dataset is extracted. The refinement remains challenging, with high R-values and displacement ellipsoids that may behave badly. The limitation of the conventional x-ray programs, that do not model the effect of multiple scattering due to the strong interaction of the electron beam with the sample, clearly appears. However, being able to extract structural information from such small crystallites remains worth the frustration. Moreover, using programs able to take into account dynamical scattering is possible and has shown to improve the results drastically (Palatinus *et al.*, 2017).

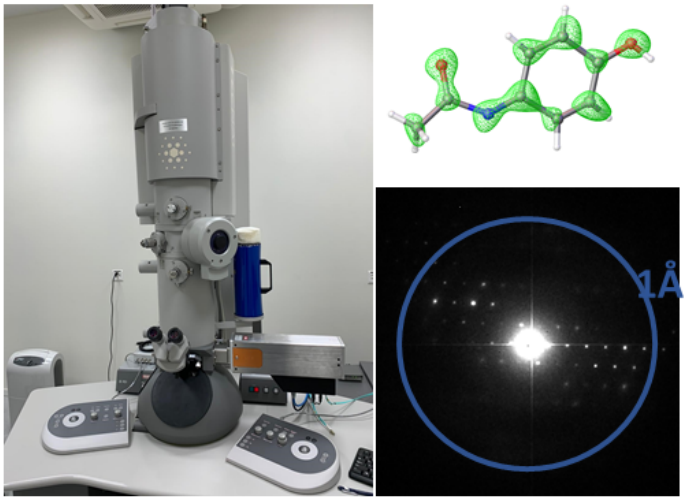


Figure 21: Our Tecnai G2 sphera equipped with a retractable 512*512 pixel hybrid pixel detector from Amsterdam Scientific. Image(0.2 deg, 0.5s) and Fobx maps obtained for a paracetamol sample.

We are now working on improving the sample handling of delicate sample (radiation sensitive, subject to solvent loss), where we will benefit from the prior experience and the equipment of the DCI for the handling of cryo-electron microscopy samples.

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We are very grateful to the people from the electron diffraction community, which have always been very helpful and eager to share their knowledge. We would especially like to thank Lukas Palatinus for organizing the ad-hoc workshops on electron diffraction and for always being so helpful. The on-line workshop on ED organized in 2021 by Xiaodong Zou's Group from the Stockholm University and their software cRed have also been of big use for us. We thank Tamir Gonen and Takanori Nakane for providing us advice via zoom. Céline and Maxime also warmly thanks Rita Therisod and Emad Oveisi from the CIME EPFL for kindly teach us about diffraction alignments in our TEM.

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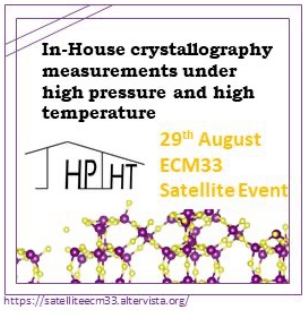

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