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

member of the scnat swiss academy of sciences

SGK / SSCr NEWSLETTER

ISSN 1662-5358 (printed edition)
ISSN 1662-534X (electronic edition)

No. 106
July 2021

From Molecules to Nanoparticles

in Biology, Chemistry, Physics and Geology

In this issue:

On the cover:
Invitation to the Annual Meeting and the General Assembly of the SGK/SSCr 2021, Sept. 2 at the Université de Fribourg.

The President's Page

Dear Members of the Swiss Society for Crystallography,

I hope that this summer edition of our newsletter finds you in good health and mood!

Time flies and my three-year term as president of the society comes to an end in September this year when I hand over this task and pleasure to the new president who will be elected at the annual meeting, organized by Katharina Fromm and Aurelien Crochet on the 2nd of September at the University of Fribourg.

During the last years we often discussed the technology-driven changes in crystallography and related sciences and how we could serve best our community in providing a platform for exchange. We conducted a review gathering information from you as members of the SSCr and will put even more emphasis on connecting scientists from different fields who nonetheless share fascination for structural research. In this regard, our society is unique!

Today, our work is dedicated to the global challenges we are facing and which are reflected in Swiss strategic focus areas related to human health, environmental and energy issues. While scientists might have their main interest in a variety of different areas, such as chemistry, physics, biology, materials science, pharmaceutical science, *etc*., and not consider themselves to be crystallographers, the SSCr presents an exciting platform for coming together to discuss, learn and exchange ideas on structural science specifically (https://sgk-sscr.ch/).

Over the last three years, we have supported a diversity of activities and highlighted electron diffraction, battery research (annual meeting 2019 in Sion, Matthew Rosseinsky as Flack lecturer in 2019), FEL and synchrotron research and not forgetting the co-organization of the SCS Symposium on Environmental Sciences 'ON THE TOP' dedicated to the Jungfraujoch Research Station which received the award 'Chemical Landmark 2019' also highlighting the early work of Max Perutz (Nobel Prize in Chemistry, 1962). Travel grants to support attendance at conferences, meetings and schools continue to be available, although much travel has been curtailed over the last 18 months. Nonetheless, we can assist also with attendance costs for participation remotely. Applications for grants are welcome.

Structural sciences continue to play an essential role in understanding viruses and in the development of drugs and vaccines; big steps forward are realized every day! In this context, we started this year an online format of our 'Howard Flack Crystallography Lecture Series' which currently emphasizes structural biology in Switzerland. Our Spring series started with speakers from renowned Swiss labs with Gebhard Schertler (ETHZ, PSI), Stefan Salentinig (Uni Fribourg) and Dimitrios Fotiadis (Uni Bern) and will continue in the Fall with Michael Hothorn (Uni Geneva), Jan Pieter Abrahams (Uni Basel) and Amedeo Caflisch (Uni Zurich).

I also hope to see you at our Annual Meeting in Fribourg. The theme will be 'From molecules to nanoparticles in Biology, Chemistry, Physics and Geology'. We look forward to talks and posters presenting new research highlights. In addition, the SSCr will award again the prize for the best PhD thesis in crystallography!

I wish to thank all of the current board members for their invaluable support during these three years. In particular, Tony Linden, who has been vice-president, Enrico Giannini who has been the treasurer of the society and Michael Wörle, who has been extremely active as secretary and editor of the newsletter. In addition, thanks to Pascal Schouwink we have now established our new website within that of the Swiss Academy of Sciences (https://sgk-sscr.ch/).

The board of the society is proposing Pascal Schouwink as new president, and I hope that the assembly will approve this decision, given that he is extremely well connected with the Swiss scientific community and a very active member of the crystallographic community. The board also proposes to confirm Enrico Giannini as treasurer and nominates Simon Grabowsky as vice-president and Antonio Cervellino as secretary. Again, I hope that the assembly will accept these nominations as this team has already worked successfully together for the last three years.

Stay curious, learn from each other and let's advance together. I wish all the best to the Swiss Society of Crystallography and will, of course, stay connected.

A safe summer time to all of you and take care!

Antonia Neels

President of the SGK-SSCr

PROGRAM Annual Meeting and General Assembly 2021

Swiss Society for Crystallography

Université Fribourg

Meeting Title:

"From Molecules to Nanoparticles in Biology, Chemistry, Physics and Geology"

Abstracts and Program

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UNIVERSITÄT FREIBURG

Thursday, September 2, 2021

Department of Chemistry, University of Fribourg
Chemin du musée 9, CH-1700 Fribourg

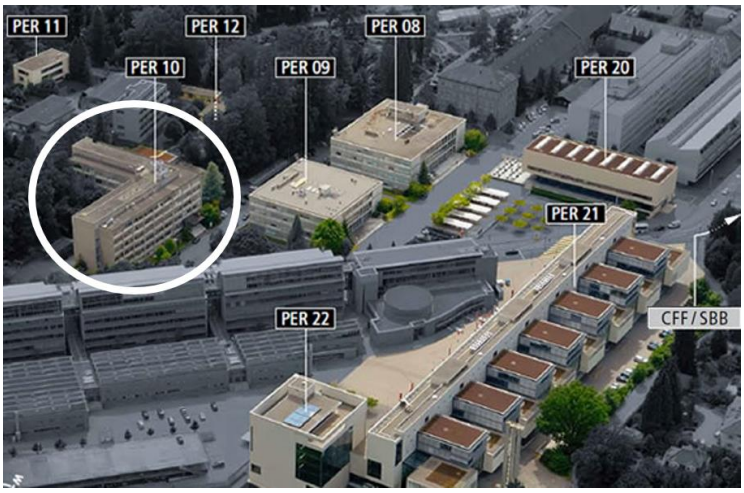
The 2021 annual meeting of the SGK/SSCr and general assembly will take place at the department of chemistry, University of Fribourg on Thursday 2nd of September 2021.
Invited speakers from academia, selected oral presentations and a poster session will show recent developments in the field.

More details on the website: http://frommgroup.ch/sgk-sscr-2021/

Registration: The meeting is free of charge (except for accommodation), however please register by email to: aurelien.crochet@unifr.ch before the 01.08.2021.

Location:

Department of Chemistry
University of Fribourg
Chemin du musée 9
CH-1700 Fribourg



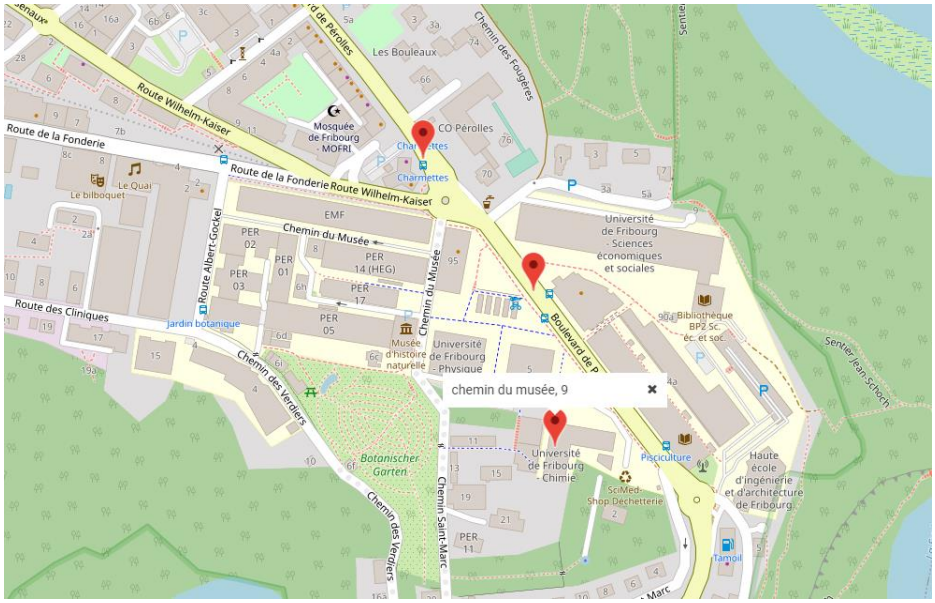
Maps and Direction:

By train: https://www.sbb.ch/en/home.html

Public transport: https://www.tpf.ch/en/#

You can stop at: “Plateau-de-Pérolles” (line 1) or “Fribourg Charmettes” (lines 3, 7 and 9).

In the picture above, you can find the Chemistry Department as PER10. If you are arriving by bus, take the bus N° 1 direction Marly until “Plateau-de-Pérolles” and walk 140m.



http://frommgroup.ch/contact-us/

9.00-10.00		Registration and Poster session
10.00-10.10	K. Fromm (UniFR) A. Neels (Empa)	Welcome messages
10.10-11.30	Session 1	Chemistry
10.10-10.50	Catherine Housecroft University of Basel	The terpyridine isomer game: ditopic and tetratopic ligands with 4,2':6',4''- and 3,2':6',3''-terpyridine metal-binding domains in metal-organic networks
10.50-11.10	Neda Iranpour Empa	Study of nanoparticles colloidal stability in biological Environment
11.10-11.30	Charles J. McMonagle SNBL	Between Single Crystal and Powder: Synchrotron Gandolfi approach for thermal expansivities and phase transitions
11.30-11.35		PhD Prize Ceremony
11.35-12.15		Invited Lecture: PhD Prize-Winner
12.15-13.40 12.50-13.40		Lunch and Posters General Assembly of the SGK
13.40-15.20	Session 2	Materials
13.40-14.20	Nicola Hüsing University of Salzburg	Hierarchically Organized Porous Metal Oxides, Carbons and Hybrids: Non-Conventional Sol-Gel Precursors and Processes
14.20-14.40	Simon Grabowsky UniBE	Development and Application of Quantum Crystallographic Methods
14.40-15.00	Kevin Schindler UniFR	Aerobically stable and substitutionally labile α-diimine rhenium dicarbonyl complexes
15.00-15.20	Samuel Watts UniFR	Virus Colloidal Interactions for Improved Water Filtration, the Importance of pH
15.20-15.40		Coffee Break and Posters
15.40-15.50		Poster Prize Winners announcement
15.50-17.30	Session 3	Biology
15.50-16.30	Robin Teufel University of Freiburg	O_2-pressurized X-ray crystallography as Tool to Study Flavoprotein Oxygenases in Natural Product Biosynthesis

16.30-16.50	Bernhard Spingler UniZH	Crystallization of small molecules with the help of robots: a new age for chemists?
16.50-17.10	Aurelio Borzì Empa	Determination of residual stress, interface degradation and lattice defects induced by an innovative packaging process: a novel HRXRD – X-ray micro CT conjoint analytical approach
17.10-17.30	Radovan Černý UniGe	Plastic crystals built from (carba-)boron clusters Lego - excellent solid-state electrolytes
17.30-19.00		Closing remarks and Aperitif

Abstracts

Oral contributions

Plenary talk (Session 1)

The terpyridine isomer game: ditopic and tetratopic ligands with 4,2':6',4"- and 3,2':6',3"-terpyridine metal-binding domains in metal-organic networks

Catherine E. Housecroft

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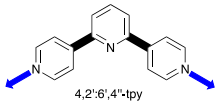
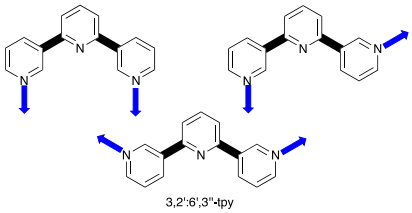
Despite the fact that the name terpyridine is synonymous with the 2,2':6',2"-isomer, there are, in principle, 47 other isomers. Not all are readily accessible synthetically, but both 4,2':6',4"-terpyridine and 3,2':6',3"-terpyridine are easily prepared and, moreover, readily functionalised in the 4'-position with coordinatively innocent or non-innocent substituents. Whereas 4,2':6',4"-tpy is restricted to being a V-shaped building block, the 3,2':6',3"-isomer is conformationally flexible:





In this presentation, we will explore the structural variation than can be achieved using the ditopic units offered by the 4,2':6',4"- and 3,2':6',3"-tpy domains with different metal nodes or linkers, and we will also show how the dimensionality of the metal coordination assemblies can be increased by moving to tetratopic domains based on covalently linked 4,2':6',4"- and 3,2':6',3"-tpy units.

Plenary talk (Session 2)

Hierarchically Organized Porous Metal Oxides, Carbons and Hybrids: Non-Conventional Sol-Gel Precursors and Processes

Nicola Hüsing [1]

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A deliberate control over the pore architecture including pore sizes, pore connectivity and tortuosity as well as pore shape is in many cases a prerequisite for their applicability, however often difficult to achieve in a laboratory [1]. Simple and general methods to prepare (functional and/or monolithic) materials with well-controlled pore architectures, composition and surface functionality are therefore highly desired.

In this presentation, sol-gel processing towards highly porous monoliths by using non-conventional sol-gel precursors and processes will be presented. This includes the application of glycolated precursors, such as tetrakis(2-hydroxyethyl)orthosilicate and the corresponding metal derivatives with and without organic monomers, as well as a discussion of the advantages but also challenges resulting from substitution of the alkoxy groups by glycoxy moieties [2].

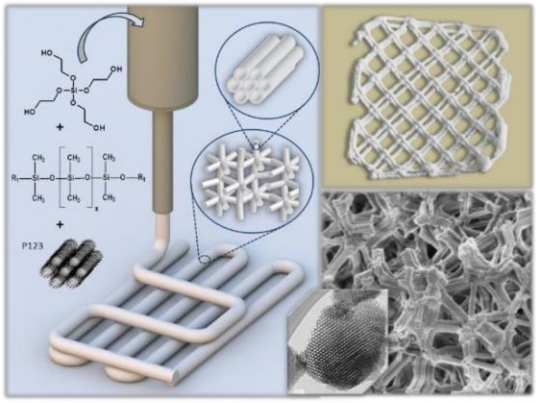

Figure 1: 3D printed hierarchically structured silica using glycolated silanes

References:

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Plenary talk (Session 3)

O_2-pressurized X-ray crystallography as Tool to Study Flavoprotein Oxygenases in Natural Product Biosynthesis

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One of the hallmark reactions catalyzed by the ubiquitous flavin-dependent enzymes is the incorporation of oxygen derived from dioxygen (O_2) into organic substrates. For many decades, these flavoprotein oxygenases were assumed to exclusively utilize the flavin-C4a-(hydro)peroxide species for oxygen transfer in monooxygenation reactions. In my presentation, I will highlight how O_2-pressurized X-ray crystallography was key for the identification of novel O_2 activation strategies in phylogenetically diverse flavoprotein oxygenases, which led to the discovery of the flavin-N5-peroxide[1] and flavin-N5-oxide[2] as novel oxygen transferring agents. Recently, a flavoprotein dioxygenase prototype could be described that even combines flavin-N5-peroxide and flavin-N5-oxide catalysis to effectuate two consecutive regio- and chemoselective oxygenations[3]. I will address how dedicated O_2 reaction sites in such enzymes control the formation of the N5-oxygen adducts and furthermore illustrate how these reactive species are employed for the redox tailoring of ecologically and pharmaceutically relevant bacterial natural products.

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Study of nanoparticles colloidal stability in biological Environment

Neda Iranpour Anaraki[1,2,3], Marianne Liebi[1,4], Quy Ong[5], Stefan Salentinig[3], Peter Wick[2], Antonia Neels[1,3*]

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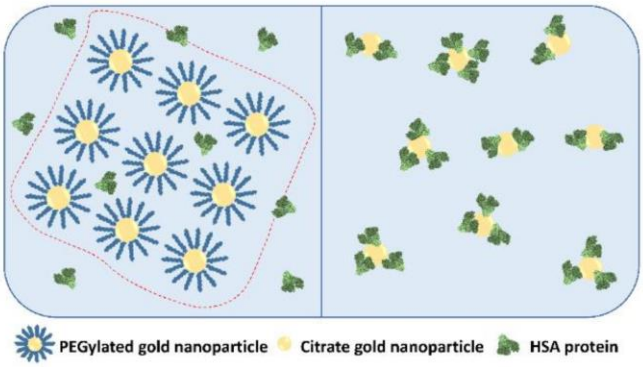
2. Laboratory of Particles-Biology Interactions, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014, St. Gallen, Switzerland
3. Department of Chemistry, University of Fribourg, Chemin du Musée, 1700, Fribourg, Switzerlan
4. Department of Physics, Chalmers University of Technology, Gothenburg 41296, Sweden
5. Laboratory of supramolecular nanomaterials and interfaces, EPFL University, Lausanne, 1015, Switzerland

Nanoparticles (NPs) bring new applications in biomedical fields. Their bio behavior is a critical issue that is strongly dependent on their colloidal stability in biological environment. Despite many investigations about dynamic and complex interactions between NPs and biomolecules, particularly proteins, these interactions are not fully understood. Small-angle X-ray scattering (SAXS), as a powerful method in NPs characterization, enables label-free in situ studies for NPs in realistic experimental environment [1]. PEGylated and citrated NPs undergo different stabilization mechanisms in biological media: we observe long-range ordering [2,3] and NP corona forming where protein molecules act as a surfactant. Our study on the NPs colloidal stability and NPs interactions with protein molecules benefits additionally from cryo-electron microscopy (Cryo-TEM), UV-Visible spectroscopy, dynamic light scattering (DLS), and zeta potential measurements. Our structural investigations enable understanding of NPs function which is essential for the future use of NPs with safe and controlled behaviors in biomedical applications.



Two different stabilization mechanisms for NPs with different surface modifications in biological environment.

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Between Single Crystal and Powder: Synchrotron Gandolfi approach for thermal expansivities and phase transitions

Charles J. McMonagle, Vadim Dyadkin, Dmitry Chernyshov

Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, 38000

Structural transition between different polymorphs in single crystals frequently leads to a degradation in crystal quality, twinning, and/or damage of crystal integrity. The most frequent reason for this is the 1st order character of phase transformations associated large latent heat and jump-like changes of unit cell volumes. In these cases, the information extracted from single crystal data by common tools can be complex and limited. Powder diffraction is not always a solution, especially if the available volume of the sample is very small due to a specificity of the material, e.g radioactivity, highly toxic, or an explosive material.
Here we present an example of Gandolfi approach [1] adapted to synchrotron diffraction experiment with area detector. The experimental diffraction data are collected with single crystal diffraction goniometry and Pilatus2M detector, where the data are treated by the Gandolfi method and analysed with powder diffraction tools. This approach, despite obvious limitations on the information content, probes the genuine in-situ structural response of initially single crystalline grain transforming via a sequence of phase transformations into a multi-domain aggregate.

Here we apply this technique to probe thermal expansion and phase transitions in the energetic material FOX-7 [2]. These data were collected at BM01 Swiss-Norwegin Beamline at ESRF, treated with the new “Gandolfi Tool” of the SNBL ToolBox software, and processed into powder-like patterns with BUBBLE [3]. Unit cell dimensions as function of temperature were refined with FullProf [4] and further analysed with PASCAL software [5].

The unit cell expansion was found to be highly anisotropic across the three phases. This can be rationalized by the anisotropic layered structure that is preserved in all three forms. Our experimentally derived thermal expansion coefficients clearly demonstrates the limitations of current theoretical estimates of thermal expansion that have been shown to be highly inaccurate, especially for the expansion normal to the molecular layers.

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Development and Application of Quantum Crystallographic Methods

PD Dr. Simon Grabowsky

Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH - 3012 Bern

The term quantum crystallography was introduced in the mid 1990's by Jerome Karle together with Huang and Massa.[1] They defined quantum crystallography as a method "for using crystallographic information with the objective of enhancing quantum-mechanical techniques and the information derived from them".[2] The actual formalism to combine diffraction experiments and theory has been developed already from the 1960's,[3] with Jayatilaka's more recent X-ray constrained wavefunction fitting technique being the most promising among the various variants.[4] However, one aspect of quantum crystallography that has only been considered for the last few years is the reverse interpretation of Karle's definition. If the wavefunction can be enhanced by the experiment, then the determination of the crystal structure can also be improved through the same quantum formalism. In this context, we will introduce the technique Hirshfeld Atom Refinement (HAR),[5] and attempt a new definition of the term quantum crystallography.[6]

For both parts of the new definition – i) the original Karle definition and ii) its reverse interpretation – we will show examples and discuss the meaning of the observed chemical effects.

i) Polarisation and electron correlation can be introduced into the wavefunction through the fitting to experimental structure factors.[7] We will show on two high-quality data sets of urea and L-alanine how these two effects can be quantified and separated in the experimental data. An extension of the same strategy might lead to the visualization of relativistic effects from diffraction data. We will show first steps into this direction.[8]

ii) HAR leads to improved accuracy and precision of crystallographic information (such as bond lengths and angles, atomic displacement parameters (ADPs) etc.). We will show how especially the treatment of hydrogens atoms benefits significantly, so that we claim that neutron diffraction experiments on small molecules will be obsolete in the future.[9]

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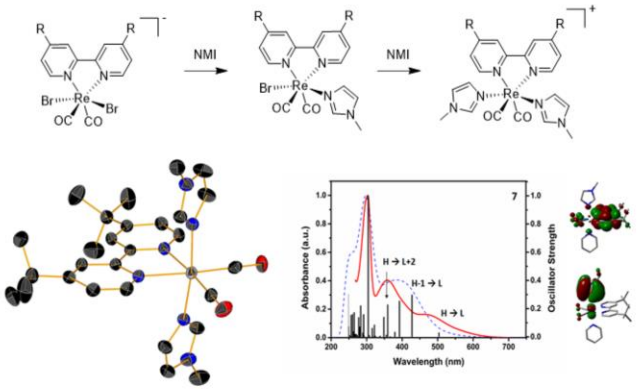
Aerobically stable and substitutionally labile α-diimine rhenium dicarbonyl complexes

Kevin Schindler, Aurélien Crochet and Fabio Zobi

University of Fribourg

New synthetic routes to aerobically stable and substitutionally labile α-diimine rhenium(I) dicarbonyl complexes are described. The molecules are prepared in high yield from the *cis-cis-trans*-$[Re(CO)_2(^tBu_2bpy)Br_2]^-$ anion (**2**, where $^tBu_2bpy$ is 4,4'-di-*tert*-butyl-2,2'-bipyridine), which can be isolated from the one electron reduction of the corresponding 17-electron complex (**1**). Compound **2** is stable in the solid state, but in solution it is oxidized by molecular oxygen back to **1**. Replacement of a single bromide of **2** by σ-donor monodentate ligands (Ls) yields stable neutral 18-electron *cis-cis-trans*-$[Re(CO)_2(^tBu_2bpy)Br(L)]$ species. In coordinating solvents like methanol the halide is replaced giving the corresponding solvated cations. $[Re(CO)_2(^tBu_2bpy)Br(L)]$ species can be further reacted with Ls to prepare stable *cis-cis-trans*-$[Re(CO)_2(^tBu_2bpy)(L)_2]^+$ complexes in good yield.[1]



*Synthetic scheme to $[Re(CO)_2(^tBu_2bpy)Br(NMI)]$ and $[Re(CO)_2(^tBu_2bpy)(NMI)_2]^+$ compounds (top), Crystal structure and UV-Vis spectra of compound **9** (bottom).*[1]

Ligand substitution of Re(I) complexes proceeds via pentacoordinate intermediates capable of Berry pseudorotation. In addition to the *cis-cis-trans*-complexes, *cis-cis-cis*- (all cis) isomers are also formed. In particular, *cis-cis-trans*-$[Re(CO)_2(^tBu_2bpy)(L)_2]^+$ complexes establish an equilibrium with all cis isomers in solution. The solid state crystal structure of nearly all molecules presented could be elucidated. The molecules adopt a slightly distorted octahedral geometry. In comparison to similar *fac*-$[Re(CO)_3]^+$complexes, Re(I) dicarbonyl species are characterized by a bend (ca. 7°) of the axial ligands towards the α-diimine unit.[1]

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Virus Colloidal Interactions for Improved Water Filtration, the Importance of pH

S. Watts[1,2], K. Maniura-Weber[1], G. Siqueira[3], T.R. Julian[4], S. Salentinig[2]

[1]Biointerfaces Lab, Empa, Swiss Federal Laboratories for Material Science and Technology, St. Gallen, Switzerland. [2]Department of Chemistry, University of Fribourg, Fribourg, Switzerland. [3]Cellulose and Wood Material Lab, Empa, Dübendorf, Switzerland. [4]Lab of Pathogens and Human Health, Eawag,Dübendorf, Switzerland

Virus contaminated water is among the leading causes of diarrheal disease outbreaks. Viruses are difficult to remove from water through conventional filtration due to their nanoscale size (with diameters < 100 nm). Adsorption filtration is a process allows to bypass this limitation of size exclusion, but requires materials that will have attractive interactions with viruses. Waterborne pathogenic viruses such as Norovirus, Rotavirus are non-enveloped viruses. Hence, their outer layer is composed of amino acids that are ionizible by pH variation. Here we investigate the effect of pH on the colloidal interactions and the nanostructure of virus surrogates, bacteria viruses MS2 and Qbeta.[1, 2] MS2 and Qbeta both have diameters below 30 nm but different surface polarities and isoelectric point, that resemble those of Norovirus and Rotavirus, respectively. Further, we designed a cellulose based adsorption filter for virus removal and characterized the colloidal interactions between Qbeta and the cellulose filter material in suspension.[2] Small angle X-ray scattering, cryogenic transmission electron microscopy and ζ-potential measurements were used to characterize the size, shape, interactions and surface properties of the viruses, the nanocellulose fibers and their combination, within the pH range 3.0 to 9.0. Aerogels, produced from cationic modified nanocellulose, were then evaluated as filter material. Confocal Raman microscopy was used to study the aerogel structure as well as to confirm the presence of the quaternary ammonium chemical modification. Filtration experiments with virus enumeration in water were performed to evaluate their efficacy.

Bacteriophages MS2 and Qbeta's structures in water in the range pH = 7.0 to 9.0 was found to be spherical with core-shell type structure. The monodispereded particles observed at pH = 7.0 transformed to micrometer sized aggregate at pH = 3.0. The virus particles nonetheless conserve their structural integrity in the aggregates. This aggregation process was also shown to be reversible. The interactions between Qbeta and cationic nanocellulose are highly pH-dependent, with strong attractive interactions at pH ≥ 5.0 and repulsive interactions at pH = 3.0. These interactions in suspension, explain the pH-dependent removal efficiency of the designed filter. At pH = 7.0, 99.9% for MS2 and 93.6% for Qbeta are removed whereas only 17.7% are removed at pH = 3.0. These pH-dependent interaction allowed to have a pH triggered filter regeneration process. The findings on the colloidal stability of viruses in aquatic environments has implications for water treatment. The colloidal state of these infectious particles will influence the efficiency of filtration, coagulation and chemical treatment processes. The interactions found between cationic cellulose and viruses provide insight allowing to further design sustainable and environmentally friendly adsorption-based filter materials for virus removal from water, and contribute to the fundamental understanding of virus interactions with positively charged sorbents in water. pH dependent cellulose-virus composites may have also have applications as biomaterials, for example as vaccine or anti-microbial material.

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Crystallization of small molecules with the help of robots: a new age for chemists?

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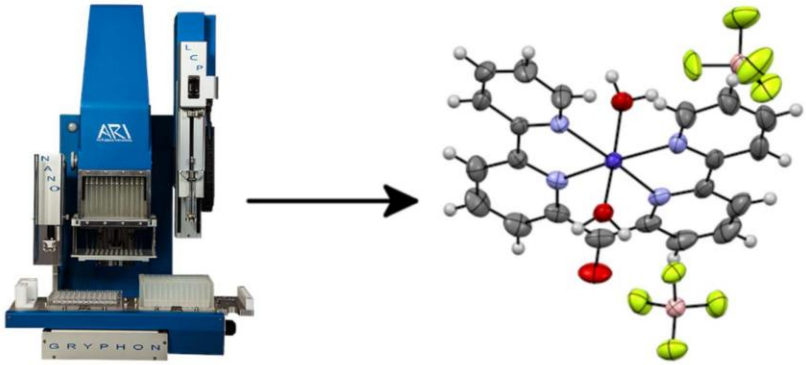
In previous years, our group has contributed to the development of "classical" crystallization of molecular compounds.[1] The term "classical" is used for a manual, individual setup of every single crystallization setup. Subsequently, we have applied the commonly used robotic approach for the growth of protein crystals[2] to the single crystal growth of small molecules. We developed a novel anion screen for this purpose, which allowed the crystallization of organic cations[3] and metal complexes[4].



During the presentation, we will discuss the advantages and disadvantages of our novel method.

We thank the University of Zurich and the Swiss National Science Foundation for financial support.

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Determination of residual stress, interface degradation and lattice defects induced by an innovative packaging process: a novel HRXRD – X-ray micro CT conjoint analytical approach

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The wafer level packaging is a key process in the fabrication of MEMS and NEMS. An adequate level of protection of the active parts of devices from the environment is accomplished only when the packaging fulfil requirements such as the hermeticity, to be maintained all long the device timelife, and low residual-stress, which otherwise may translate into bending, deformations, nonlinearities and failure [1], [2]. A novel wafer-level packaging technique, namely impulse current bonding (ICB), potentially takes advantages over the well-established silicon to glass anodic bonding (AB) technology in terms of its suitability for the bonding between a wide class of materials, from ceramics to metal, and outstanding limitation of the process-temperature, consequently reducing the residual stress. Here a comparison between ICB and AB packaging is presented. The extreme strain-detection-power of high-resolution XRD enabled to investigate the residual stress in the c-Si single-crystals bonded with the borosilicate-glasses [3]. The presence of lattice defects is also quantitatively evaluated. The X-ray micro-CT visualization of the bonding interfaces enabled to assess about the presence of micron-sized defects, such as cracks and voids. This work represents a first milestone toward the assessment of the ICB-process reliability and the full-comprehension of the associated bonding mechanism.

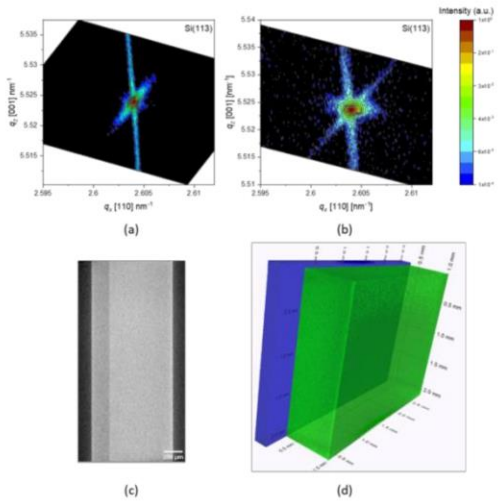

Figure caption: Distribution of the scattering vector intensity in the reciprocal space for the 113 reciprocal lattice point (RLP) of c-Si. (a) Anodic Bonding processed sample; (b) Impulse Current Bonding processed sample. X-ray micro computed tomography images of Si/glass ICB-processed samples. (c) high-resolution cross section; (d) 3D rendering of the bonding interface.

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Plastic crystals built from (carba-)boron clusters Lego - excellent solid-state electrolytes

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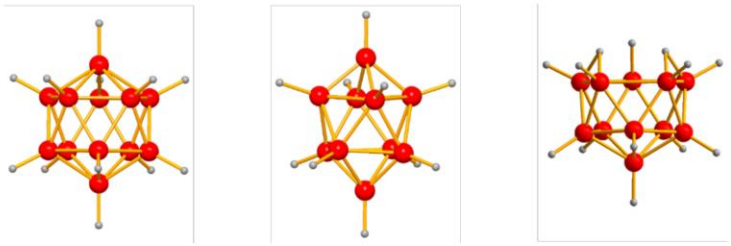
Complex hydrides were deeply investigated for solid-state hydrogen storage, and since few years also as solid-electrolytes [1]. Li and Na salts based on various *closo*- and *nido*- hydrogen-(carba-)boron clusters are among the best (Figure 1). Elevated ionic motion occurs only after a structural phase transition leading to rotatory plastic crystal, *i.e.* rotating clusters, which generally occurs beyond room temperature (*rt*). Frustrating the anion sublattice, either by anion replacement or anion mixing, is an effective strategy to stabilize down to *rt* the conductive phase. Playing with the (*carba*-)boron clusters Lego allows to vary the parameters controlling the ionic conductivity: cation content in the crystal, cluster packing type (*ccp*, *hcp*, *bcc*) and order/disorder transition temperature [3].

Following this approach, we discovered $Na_4(CB_{11}H_{12})_2(B_{12}H_{12})$ featuring a superior ionic conductivity σ = 2 mS cm^{-1} at *rt*, with a low activation energy of 314 meV [2]. Electrochemical stability of 4.1 V vs. Na^+/Na is compatible with high-voltage operating positive electrodes [4,5].



Icosahedron
$B_{12}H_{12}^{2-}$
$CB_{11}H_{12}^{-}$
$C_2B_{10}H_{12}$

Bi-capped square antiprism
$B_{10}H_{10}^{2-}$
$CB_9H_{10}^{-}$

Open cage
$B_{11}H_{14}^{-}$

Figure 1: Panoplie of (carba-)boron clusters Lego.

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Poster contributions

How X-Ray diffraction can be useful for the stress evaluation of watchmaking rubies?

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In a watch movement, small rubies are press-fitted into the plate and bridges (generally in brass) to form low-friction bearings for the gear wheels. This press-fitting process is sensitive and controlling the quality of the assembly is difficult. This study is focused on evaluating the quality of the press-fitting process by analyzing the stress induced in the rubies. The level of stress is measured by high resolution X-Ray diffraction in combination with the fluorescence spectroscopy. A steel plate containing 30 rubies (torus shape of 1.6 mm diameter) press-fitted with increasing interference (max. 15 µm) is used as a test sample (**Fig. 1**).

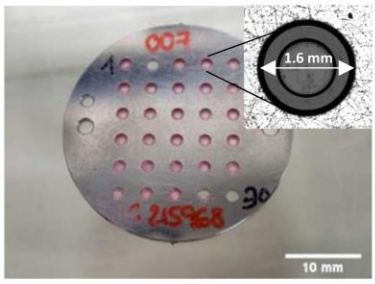

Fig. 1 *Steel plate containing 30 press-fitted rubies. Press-fitting interference is increasing with ruby number.*

The obtained results will demonstrate how X-ray diffraction and fluorescence spectroscopy can be used to assess the induced stress in the ruby parts. High resolution XRD measurements were carried out for the non-destructive quantitative analysis of the stress in ruby parts. The reciprocal space measurements (RSM) were performed on the Al_2O_3 (113) reflections. The stress value was calculated from the shift and distortion of the RSM peak with respect to a stress-free reference ruby piece. Fluorescence spectroscopy has been conducted on each ruby at the 4390 cm^{-1} peak. A shift of the peak position towards higher wavenumbers indicates higher stress in the material [1].

The results obtained by XRD and fluorescence spectroscopy exhibit a good correlation and show that rubies with higher interference exhibit stronger stresses. Quantitative XRD data can be used for calibration of the fluorescence spectroscopy results. This study has shown the direct application of HR-XRD for industrial needs.

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Lattice strain and defects analysis in semiconductor materials by means of HRXRD methods

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Crystal lattice stress/strain, aging, degradation, and reliability are important topics in semiconductor materials and devices. In new semiconductor materials, stress/strain is often used as a design element for improving the mobility of electrons [1]. High-resolution X-ray diffraction (HRXRD) is a sensitive and non-destructive technique for analyzing the crystal lattice strain in quasi-perfect and structured crystalline materials such as nanowire systems [2], thin films [3], and more complex nano- and microelectromechanical systems (NEMS, MEMS) [4]. Lattice deformation is mainly caused by the presence of defects such as dislocations and point defects, which are introduced during fabrication or under the device working conditions. Here, we show different experimental (synchrotron and lab-source) and analytical (2- and 3D reciprocal space mapping) approaches to investigate the mechanisms of lattice defects occurrence and their mobility. We studied single-crystal silicon nanowires (SCSi NW) for sensing applications, single-crystal diamond micromechanical components for photonic devices, single-crystal sapphire for watch components [5], and $BaTiO_3$ thin films for sensing and energy storage applications.

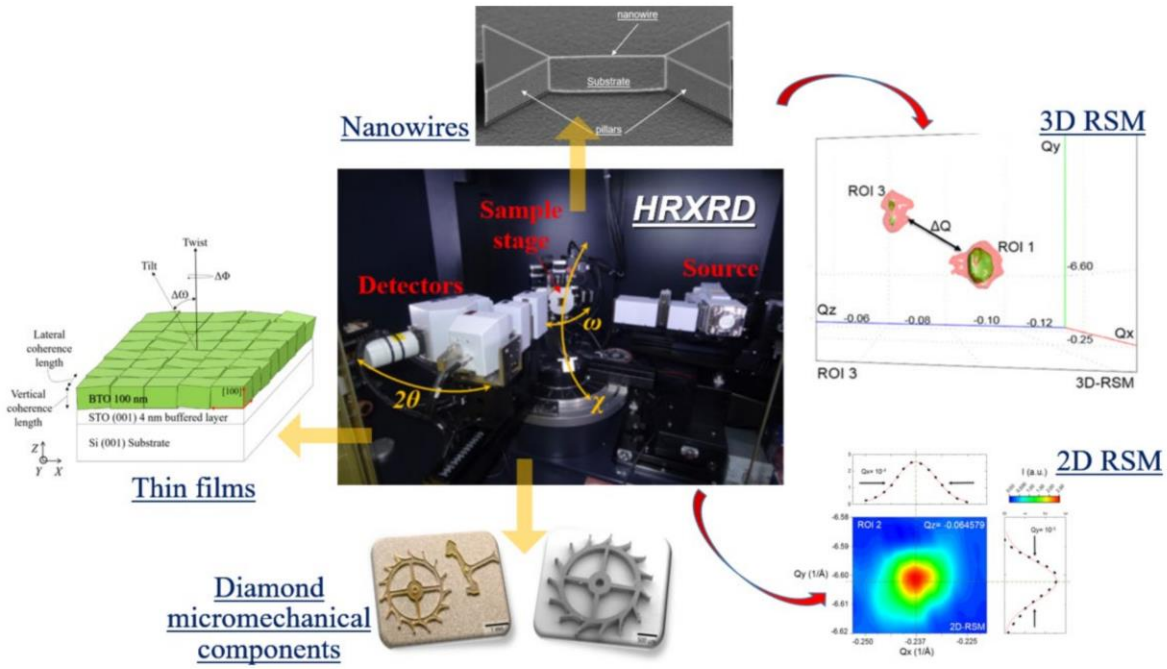

Figure: HRXRD methods for lattice strain and defects analysis of semiconductor materials and devices.

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MgO-based CO_2 sorbents: formation of $MgCO_3$ at the buried $NaNO_3$-MgO interface investigated by X-ray grazing incidence diffraction, reflectometry, and electron microscopy

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MgO-based CO_2 sorbents promoted with molten salts are emerging materials for carbon dioxide capture and storage (CSS) applications. [1] So far, mostly trial-and-error-based approaches have been utilized to improve the CO_2 capture performance of this class of sorbents. These works focused largely on optimizing the promoters' composition, introduction of additional nucleation seeds or MgO with differing morphologies. [2] It has been found that bare MgO is almost inactive for CO_2 capture, yet when promoted with molten alkali salts, high rates of CO_2 capture through the formation of $MgCO_3$ are obtained. Yet there is still no in depth understanding of the mechanism of $MgCO_3$ formation in molten-salt-promoted MgO sorbents. A key information that is required to understand how these sorbents function is therefore: how and where $MgCO_3$ forms. To answer this question, we have investigated a well-defined model system of a MgO(100) single crystal coated with $NaNO_3$ as well as a pristine MgO(100) single crystal using X-ray- and electron-based characterization tools. [3]

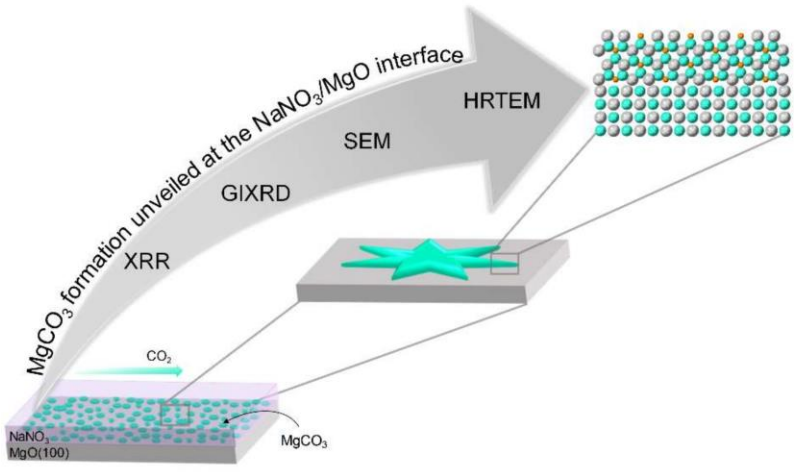

Figure 1. Schematic illustrating the use of in situ X-ray and ex situ electron microscopy techniques to provide micron to atomic scale insight into the formation and growth of $MgCO_3$ during CO_2 capture at the $NaNO_3$/MgO(100) interface.

To characterize the MgO(100) surface and $NaNO_3$/MgO(100) interface at relevant carbonation and calcination conditions we have used synchrotron-based in situ X-ray reflectometry (XRR) and grazing incidence X-ray diffraction (GIXRD). XRR allowed us to determine that for a pristine MgO(100) crystal carbonation is limited to a layer with the thickness of ca. 7 Å, i.e. largely limited to surface carbonation. On the other hand, $NaNO_3$-promoted MgO(100) exhibited a drastic increase in the surface roughness upon exposure to CO_2. As confirmed by GIXRD, the surface roughening is due to the formation of (micron sized) $MgCO_3$ crystals at the interface between the MgO (100) crystal and the molten salt. Noteworthy, the $MgCO_3$ crystals formed were highly oriented with respect to the MgO(100) substrate. The morphology of the $MgCO_3$ product was investigated further by scanning electron microscopy (SEM), showing that the $MgCO_3$ crystals exhibited a two-dimensional sectored plate morphology (size of 10-50 µm; thickness of 2 µm), which is in line with a heterogonous nucleation mechanism of $MgCO_3$. Furthermore, high resolution transmission electron microscopy (HRTEM) of a lamella cut parallel to the (100) plane of the MgO substrate provided insight into the atomic arrangement at the $MgCO_3$/MgO interface, revealing that $MgCO_3$ growth is epitaxial with respect to the MgO(100) crystal. The large lattice mismatch between $MgCO_3$ and MgO is relaxed through the introduction of lattice misfit dislocations.

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Proposed international standard for magnetic space-group numbers and symbols

IUCr Commission on Magnetic Structures

& Hans Grimmer

Paul Scherrer Institute

To address long-standing weaknesses in the Belov-Neronova-Smirnova (BNS) and Oppe-chowski -Guccione (OG) symbols for magnetic space groups (MSGs), a new international (INT) system of MSG numbers, symbols, and crystallographic settings is proposed. The INT system is a modification of the BNS system, having the same crystallographic settings, but different numbers and symbols.

Although the author is not a member of the commission, he was invited to contribute to the proposition.

Case	BNS #	BNS	OG #	OG	INT #	INT	MPG
[1]	2.7	$P_S\bar{1}$	2.4.7	$P_{2s}\bar{1}$	7	$P\bar{1}.1'_I[P\bar{1}]$	$\bar{1}.1'$
[2]	42.223	F_Smm2	25.9.163	P_Imm2	321	$Fmm2.1'_I[Pmm2]$	$mm2.1'$
[3]	146.12	R_I3	146.3.1242	R_R3	1242	$R3.1'_c[R3]$ hex $R3.1'_I[R3]$ rhomb	$3.1'$
[4]	218.84	$P_I\bar{4}3n$	217.5.1584	$I_P\bar{4}'3m'$	1586	$P\bar{4}3n.1'_I[I\bar{4}3m]$	$\bar{4}3m.1'$
[5]	140.550	I_c4/mcm	123.19.1017	$P_I4/mm'm'$	1210	$I4/mcm.1'_c\ [rP4/mmm]$	$4/mmm.1'$
[6]*	28.96	P_Bma2	39.7.284	A_Pbm2	194	$Pma2.1'_B[Bma2]$	$mm2.1'$
[7]	1.1	$P1$	1.1.1	$P1$	1	$P1.1$	1.1
[8]	1.2	$P11'$	1.2.2	$P11'$	2	$P1.1'$	$1.1'$

*$A_Pbm2 \rightarrow Abm2 \rightarrow Bma2$

The BNS, OG, and INT symbol are given for each MSG example, as well as the corresponding magnetic point group (MPG) symbol (with separation of magnetic and non-magnetic generators).

To obtain an unambiguous anti-translation subscript in the BNS-system

the subscript "S" has been replaced with "I" for triclinic MSGs and for orthorhombic MSGs for which the maximal space subgroup has a face-centered conventional cell (examples 1 and 2).

For rhombohedral groups, the subscript "c" should be used in a hexagonal-axis setting, while the subscript "I" should be used for a rhombohedral-axis setting (example 3).

In summary, the unambiguous INT subscripts are: "a" = (1/2,0,0), "b" = (0,1/2,0), "c" = (0,0,1/2), "A" = (0,1/2,1/2), "B" = (1/2,0,1/2), "C" = (1/2,1/2,0), and "I" = (1/2,1/2,1/2).

The MPG is obtained from the INT symbol simply by removing any translational detail from each generator given in INT (examples 1-8).

The INT symbol moves the subscript from the BNS lattice-centering character to the time-reversal generator symbol (examples 1-6).

Texture and Total Scattering

Antonio Cervellino[a] and Ruggero Frison[b]

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(b) University of Zurich, Zurich, Switzerland

Texture (preferential orientation) invalidates THE basic assumption of powder diffractometry – that the sample is constituted of a set of many identical particles (individual micro- or nanocrystals) differing only in orientation, in a perfectly random fashion, with a spherically isotropic orientation distribution function (ODF). Deviations from this ideal isotropy are named texture.

Considerable work [1] has been done in the past to quantify the effects of texture on the Bragg peaks intensities. Much less if anything has been done to quantify general effects on the pattern, concerning e.g. the diffuse background of crystalline systems or major parts of the pattern of less/not crystalline objects, that can be today profitably studied by Total Scattering (TS) methods. The basis of TS is the Debye scattering equation (DSE), which always yields the complete powder pattern. We, therefore, have developed a generalized form of the DSE [2] that includes texture effects, described in the Spherical Harmonics framework, accounting for the full list of subcases for different symmetries of the sample and the three most common experimental geometries (Debye-Scherrer capillary (DS), Bragg-Brentano flat plate (BB) and flat-plate transmission (FP)). Moreover, we have investigated the effect of texture on Pair Distribution Function (PDF) analysis, with some important caveats – texture can be as destructive within the PDF pattern in direct space as it is in reciprocal space.

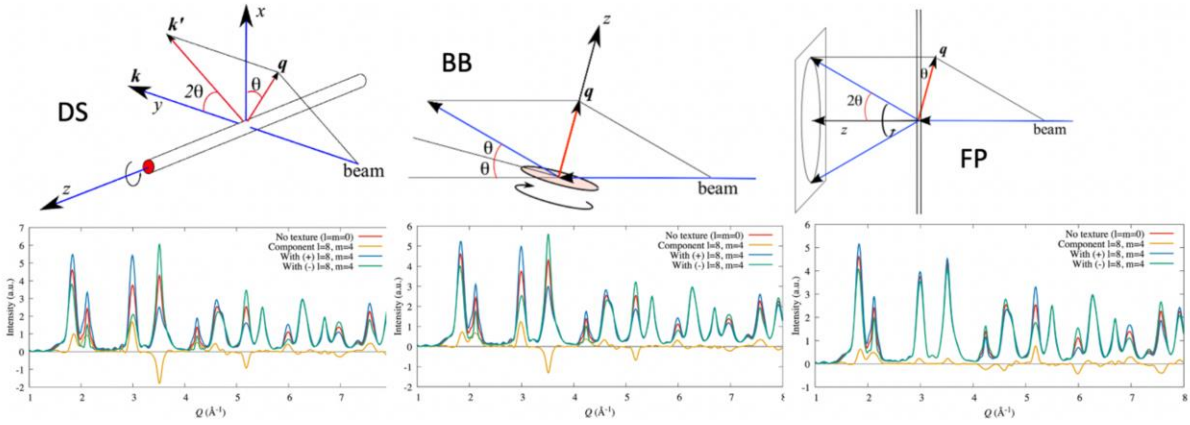

Figure caption:

The three most common experimental geometries (DS, BB, FP) and the depiction of the effect of a single continuous texture component (here *l*=8, *m*=4) calculated by the DSE generalized for texture in a simple powder pattern of cubic nanocrystals.

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Design, synthesis and *in vivo* evaluation of 3-arylcoumarin derivatives of rhenium(I)tricarbonyl complexes as potent antibacterial agents against methicillin-resistant Staphylococcus aureus (MRSA)

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The increase of antimicrobial resistance (AMR) to current clinical drugs and the lack of new antibiotics to combat emerging resistant strains have become major concerns to human health in this century.[1-3] Among the all strains, methicillin-resistant *Staphylococcus aureus* (MRSA) represents the leading cause of nosocomial and community-acquired infections, being recognized by the World Health Organisation (WHO) as the antibiotic-resistant pathogen of high priority. Therefore, a high demand for novel therapeutic options to combat MRSA-related infections.[4-5]

We have prepared a series of ten 3-arylcoumarin molecules, their respective *fac*-$[Re(CO)_3(bipy)L]^+$ and *fac*-$[Re(CO)_3(N^{\frown}N)Br]$ complexes and single-crystal X-ray structure of some ligands and complexes such as L_1, L_2, L_5, L_6, L_8, ReL_2, ReL_5 and ReL_7 (shown in Fig. 1 and Fig. 2). All species were tested for their antimicrobial efficacy. Whereas the 3-arylcoumarin ligands are virtually inactive against the human-associated pathogens with minimum inhibitory concentrations (MICs) > 150 µM, when coordinated to the *fac*-$[Re(CO)_3]^+$ core, most of the resulting complexes showed remarkable antibacterial potency. Several rhenium complexes exhibit activity in nanomolar concentrations against Gram-positive pathogens such as *Staphylococcus aureus* strains, including methicillin-resistant *S. aureus* (MRSA) and *Enterococcus faecium*. The molecules do not affect bacterial cell membrane potential, but some of the most potent complexes strongly interact with DNA, indicating it as a possible target for their mode of action. *In vivo* studies in the zebrafish model showed that the complexes with anti-staphylococcal/MRSA activity were non-toxic to the organism even at much higher doses of the corresponding MICs. In the zebrafish-MRSA infection model, the complexes increased the survival rate of infected fish up to 100 % and markedly reduced bacterial burden. Moreover, all rescued fish developed normally following the treatments with the metallic compounds.

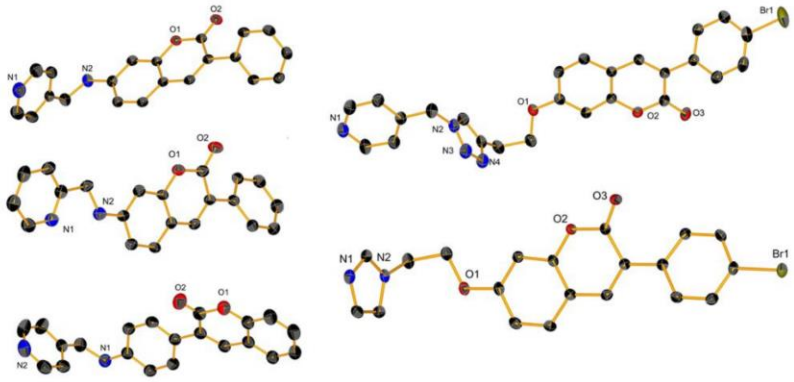

Figure 1. Ortep representation of left: (from top to bottom) ligands L_1, L_2, L_5, and right: (from top to bottom) L_6 and L_8. Thermal ellipsoids set at a 30% probability level. Hydrogen atoms, as well as solvent for L_2, are omitted for clarity.

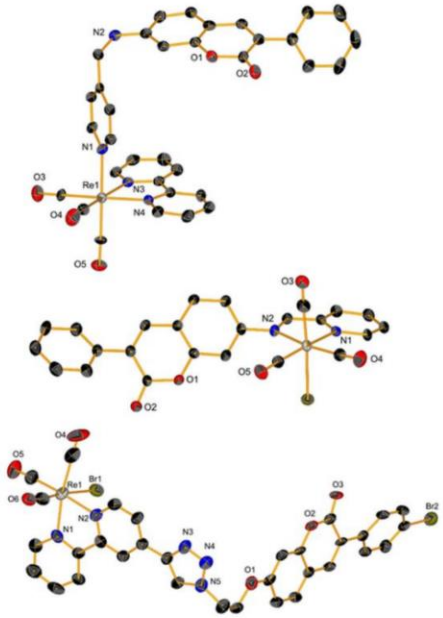

Figure 2. Ortep representation of (from top to bottom) ReL_2, ReL_5 and ReL_7. Thermal ellipsoids set at a 30% probability level. Hydrogen atoms, as well as solvent and counter ion for ReL_2 and minor partitioning for ReL_5 and ReL_7, are omitted for clarity.

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BM01 station of Swiss-Norwegian Beam Lines: current status and near future.

Vadim Dyadkin, Dmitry Chernyshov, J. McMonagle and Wouter van Beek

Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, 38000

BM01 is a diffraction station focused on crystallography with single crystal, powder diffraction, and thin films. The station performs a large range of in-situ and operando experiments with users from different branches of material science and is one of the most productive beamlines at ESRF.

Here we show the status of the beamline with a list of currently available experimental conditions and present future development for sample environments. We also discuss the near future development of the station. These include an upgrade of the primary detector for diffraction experiments, the re-location of the diffractometer to allow for small-angle scattering experiments, and the modification of the monochromator to improve beam stability.

We also present the dedicated custom beamline software that is essential to make experiments on BM01 both very flexible and user-friendly. The inhouse developed software includes data manipulation, processing and visualizations tools. These tools allow users to start working on the crystallography, physics, or chemistry of their materials as soon as the images leave the detector.

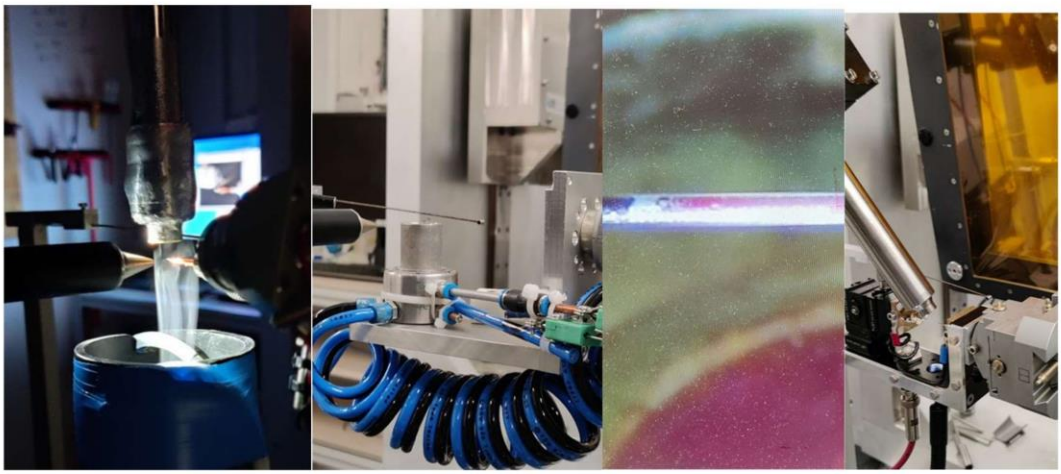

Fig. 1. From left to right: single crystal diffraction at 10K, thin film heating cell, capillary with powder at high temperature, single crystal cell for electric field and temperature -dependent diffraction experiments.

Radiation Damage in Small Molecule Crystallography: synchrotron experiments with an organic ferroelectric and a spin crossover complex.

Dmitry Chernyshov

Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, 38000

Fast area detectors and bright synchrotron sources make possible to follow evolution of crystals structures as a function of external stimulus, like temperature, pressure, electric or magnetic field. The most detailed information can be obtained from single crystal diffraction measured with a fine step in the field and this unavoidably implies many datasets to measured and analyzed. The use of high flux X-ray radiation from synchrotrons may lead to a progressive accumulation of the radiation damage even for small molecules. The effect of which has become more severe and more frequently observed with the latest generation of synchrotron sources with enhanced brightness, e.g. EBS at ESRF.

Here we consider two representative examples from the field of single crystal experimentation at BM01 Swiss-Norwegian Beamline [1]. First example is an organic ferroelectric, Glycinium phosphite. The thermal evolution of Glycinium phosphite was probed by single crystal diffraction with both synchrotron radiation and a laboratory X-ray diffractometer [2]. Both measurements showed a transition from paraelectric to ferroelectric state at nearly the same temperature, T_C= 225 K. However, the evolution of the unit cell parameters and volume with temperature are drastically different for data collected at the synchrotron and laboratory. The latter case corresponds to the previous reports and shows the expected contraction of the cell on cooling. Whereas an abnormal, non-linear increase of unit cell volume on cooling is seen with data collected at the synchrotron.
Our second example is on the effect of the radiation damage to the spin state conversion in a Fe-based spin crossover complex, where we characterize the kinetics of radiation damage with time-resolved single crystal diffraction [3]. We also observe a radiation-induced increase of the unit cell volume that, for spin-crossover materials, affects the conversion between spin stated.

Here, we discuss different strategies for single crystal data collections to minimize the radiation damage and the observed effect of the radiation on the macroscopic properties such as polarization and magnetic susceptibility.

References

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Quantum crystallographic evaluation of the YLID crystal structure; reconsidering calibration of x-ray diffractometers

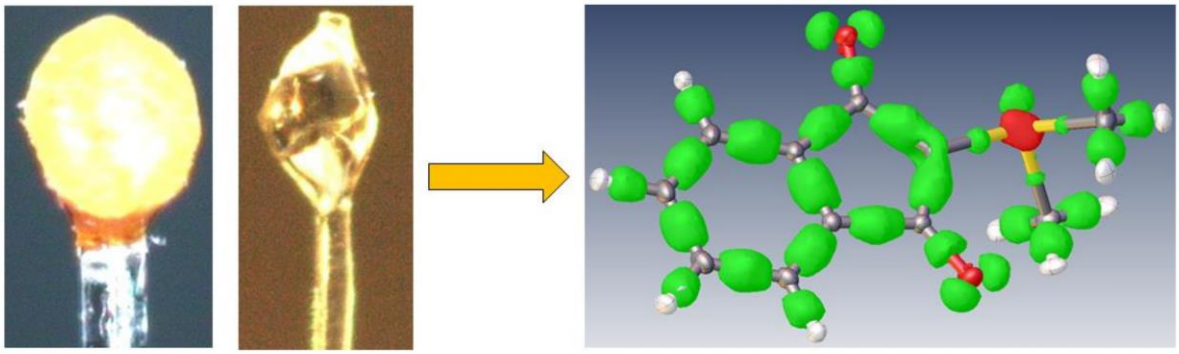
Yaser Balmohammadi,[1] Lorraine A. Malaspina,[1] Milosz Siczek,[2] Simon Grabowsky[1]

1 Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Switzerland

2 University of Wroclaw, Faculty of Chemistry

Since 1969, YLID crystals have been routinely used as test crystals for X-ray diffractometers. YLID is stable at room temperature, crystals could easily be ground to spheres, its small unit cell (ca. 1000 Å^3), and orthorhombic symmetry are advantegous properties for an off-the-shelf test system. Therefore, the crystal structure has been determined innumerable times.[1] Despite that, no charge density measurement has been performed for this test system. It is certainly more meaningful if we compare the (readily available) charge density distribution after each calibration instead of average intensities or internal R-values.

In this study, the crystal structure of the YLID test crystal for X-ray diffractometers is studied under different conditions. The data for the study were collected using three different wavelengths (Cu=1.54184 Å, Mo=0.71073Å, Ag=0.56087Å) and three different temperatures (272K, 150K, 100K). The YLID experimental electron density was obtained using multipole refinement[2] and X-ray wavefunction refinement[3]. Our results demonstrate that for the calibration of a diffractometer, the usual x-ray analysis of YLID test crystal is not enough and quantum crystallographic studies should be performed.



Quantum crystallographic analysis of YLID test crystal

References

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Non-Spherical Atoms in Crystallographic Models

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The crystallographic model of a structure is the key in the interpretation of diffraction patterns, understanding of molecular structure and predictions of properties like pharmaceutical activity or material properties. With modern detectors and bright X-ray sources more features of the diffraction pattern are observed that cannot be explained using the well-established Spherical or Independent Atom Model (IAM). The implementation of a common interface to allow the use of non-spherical atomic form factors from any model or software in NoSpherA2[1] allows standardized use of non-spherical models to refine and analyze routine X-ray and electron diffraction structures employing the most suited model of atomic form factors matching the structure at hand. This makes Quantum Crystallography[2] more accessible to the whole crystallographic community.

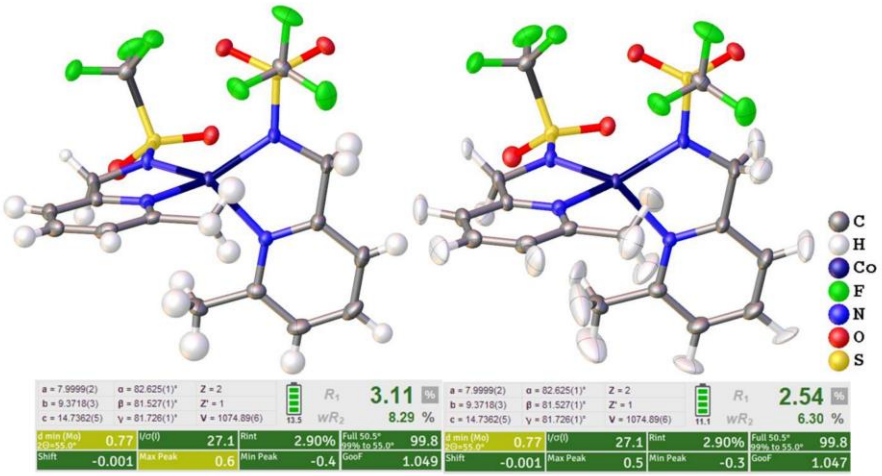

Figure caption: Spherical Atom Model (left) and Non-Spherical-Atom-Refinement (right) with model visualization (top) and refinement statistics (bottom).

In addition to better refinement statistics, the non-spherical refinement can yield accurate hydrogen atom positions from X-ray diffraction data and higher precision on all atom positions and distances, due to the better description of the measured data. This presentation will show the benefits and possible applications available using non-spherical models from classical salts towards biochemical applications in rational drug design using the Hirshfeld Atom Refinement [3] model as an example.

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lamaGOET: an interface for quantum crystallography

Lorraine A. Malaspina, Simon Grabowsky

Department of Chemistry, Biochemistry and Pharmaceutical Sciences, Universität Bern.

The use of quantum chemistry concepts and calculations in crystallographic refinements provides a new promising path for more accurate structure determination; this is the field of Quantum Crystallography (QCr). [1] One of such QCr techniques is Hirshfeld Atom Refinement (HAR) [2,3] which was initially introduced in the program Tonto, a program and library for quantum crystallography and quantum chemistry.

Despite its availability, the use of Tonto usually requires expertise beyond regular ShelXL-type structure refinement and knowledge of its program implementation. Example input files to the many different functionalities available in the software can be found in the "tests" folder provided with the software installation, however, building your own input files is not such a trivial task, especially when using more advanced functionalities of experimental electron-density (ED) research [4,5].

The lamaGOET interface not only provides a graphical interface which creates and runs the necessary inputs for Tonto jobs related to HAR, but also allows the use of more advanced experimental ED features inside Tonto such as X-ray Constrained Wavefunction (XCW) fitting [4] and X-ray Wavefunction Refinement (XWR = HAR + XCW) [5]. The XCW procedure allows access to the "experimental" wavefunction and therefore an experimentally derived electron density.

In HAR, a quantum-mechanical calculation needs to be performed at every refinement step in order to obtain the theoretical electron density which is used to derive aspherical tailor made scattering factors. Therefore, in addition to the previously mentioned functionalities, the lamaGOET graphical interface integrates the option for the user to perform a HAR using different quantum chemistry softwares of their choice such as Gaussian, Orca, ELMOdb or the original Tonto.

In this work, we present how to use the lamaGOET interface to perform such refinements and fittings and how to analyze the results through the calculation of different properties using the derived wavefunctions.

References

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Crystal structure of new polymorph of Sr_2TiO_4 with tetrahedral titanium

D. Pulmannova[1], C. Besnard[1], E. Giannini[1]

1 Univeristy of Geneva, Quai Ernest-Ansermet 24, 1205 Geneva, Switzerland

Sr_2TiO_4, first member of the Ruddlesden-Popper series $Sr_{n+1}Ti_nO_{3n+1}$, has been long known to undergo a phase transition at 1550 °C. This transition makes the growth of single crystals of this material highly challenging, because it usually breaks the crystal into a periodic array of uneven lamellae. While the low temperature tetragonal phase is widely studied due to its close connection to the famous perovskite $SrTiO_3$, there is little information about the high temperature α-phase, except for an unindexed powder pattern by Drys&Trzebiatowski [1].

We stabilized the high-temperature α-Sr_2TiO_4 crystals by rapid cooling of the incongruent melt from above the liquidus temperature. The α-phase crystallizes in the orthorhombic $Pna2_1$ group with lattice parameters a=14.2901(5) Å b=5.8729(2) Å c=10.0872(3) Å and is isostructural to the orthorhombic forms of Sr_2VO_4 and Sr_2CrO_4 (which belong to the β-K_2SO_4 structure type). Its structure is formed by a complicated framework of large SrO_x polyhedra with tetrahedral cavities occupied by the transition metal. The tetrahedral coordination of Ti^{IV} makes the α-Sr_2TiO_4 quite a rare case among titanate compounds, the only other known example being the barium orthotitanate Ba_2TiO_4 [2].

However, whereas in Ba_2TiO_4 the coordination is tetrahedral in both high- and low-temperature polymorphs and the topotactic relation between the two is known, in the case of Sr_2TiO_4 a transition occurs to the layered Ruddlesden-Popper structure with octahedral titanium coordination.

In this work, we report for the first time the crystal structure of the high-temperature α-phase of Sr_2TiO_4. We elucidate the structural differences between the related compounds and discuss possible mechanism driving the structural transition.

References

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Macrocyclic Ligands: From Synthesis Towards On-Surface Topology, and their Candidacy as Synthons for Interlaced Structures

Ali Kaiss,[a] Antoine Hinaut,[b] Aurélien Crochet,[a] Ernst Meyer,[b] Katharina M. Fromm[a,*]

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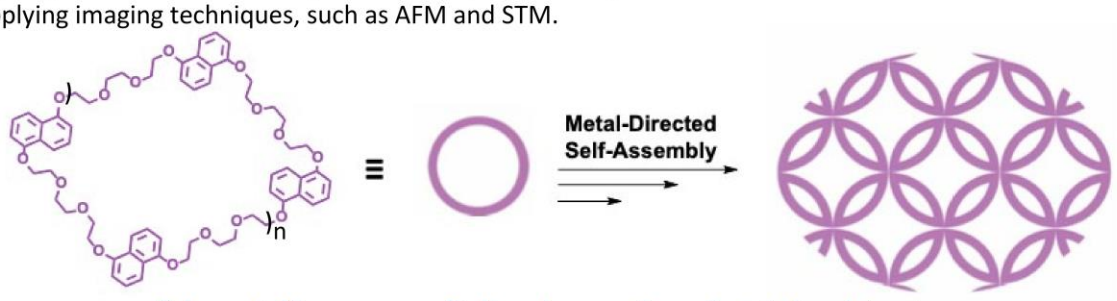
[b] Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Knots and links, being part of the mechanically interlocked molecular architectures, are related to three-dimensional space (manifolds). Nevertheless, links are less studied and are not as well classified as knots.[1] Nature shows examples of strong relations between topology and function;[2,3] for instance, complex topological structures such as those present in the chain mail-like armour lying under Komodo warren's skin are extremely robust,[4] as is the structure forming the capsid of the virus HK97.[5]
To achieve chain mail type structures, macrocycles need to interlink with each other. Such complex topologies of links can be analyzed for example by looking at them at the atomic level. This is achieved by applying imaging techniques, such as AFM and STM.



Scheme 1: New macrocyclic ligands as synthons for interlaced structures

New synthons, like a new family of macrocycles with alternating aromatic and polyether chains, have been synthesized and characterized with the aim of obtaining complex chain-mail structures (Scheme 1). These flexible and robust macrocyclic structures are formed by alternating the mechanical and physical properties resulting from the different building blocks. Their arrangement on atomically flat 2D structures have been investigated and compared with the 3D-structures obtained from single crystal analyses.

References

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3D Electron diffraction for the discovery of new crystal forms of APIs

A. E. Lanza[1], J. Potticary[2], C. Hall[2], V. Hamilton[2], S.R. Hall[2], G. Santiso-Quinones[1], E. Hovestreydt[1]

[1]ELDICO Scientific AG, 5234 Villigen, Switzerland,
[2]School of Chemistry, University of Bristol, Bristol, BS8 1TS, United Kingdom

3D Electron diffraction (3D ED)[1] has recently emerged as a powerful tool for the discovery of new crystalline forms of pharmaceutical compounds,[2-4] as it allows to bypass many of the common bottlenecks of this process and of the established characterization methods based on x-ray diffraction. Small crystal size, mixture of phases, small product quantities are very frequent obstacles to the structural characterization of APIs that can be easily overcome by 3D ED methods.

Here we showcase how our electron diffractometer, fully dedicated to 3D ED experiments, represents a revolutionary innovation for the discovery of new crystal forms of APIs. Our recent results of representative case studies dealing with challenging pharmaceutical compounds will demonstrate the performances of a dedicated device and how it can meet the growing needs of the crystallographic and pharmaceutical community.

References

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Swiss Crystallographic Association SGK / SSCr

General Assembly 2021

Thursday, September 2, 2021, 12:50-13:40
Department of Chemistry, University of Fribourg
Chemin du musée, 9; 1700 Fribourg

Agenda of the General Assembly 2021

The minutes of our last General Assembly (Online meeting via ZOOM; Wednesday, September 9, 2020, 10:00 – 11:30) are published on page 44-54 of the SGK/SSCr newsletter No. 106, July 2021 (this issue), which is also available electronically at https://www.sgk-sscr.ch

1) Determination of the quorum according to Art. 12/by-laws

2) Proposal for acceptance of the minutes of the General Assembly 2020, online meeting

3) a) Annual report
   b) Annual financial statement
   c) Budget for the next year
   d) Regulation of the annual membership fees

4) a) Definition of a chairperson for the elections
   b) Confirmation of the present board members.
   c) No current nominations of new board members. Nominations should be communicated to the president 10 days prior to the meeting.
   d) Assignment of the new secretary, president and vice president: Nominations are Pascal Schouwink for president, Simon Grabowsky for vice-president and Antonio Cervellino for secretary.
   e) Election/confirmation of the auditors
   f) Election of the delegates to ECA, IUCR and IOCG

5) 2022 Meeting and General Assembly: at the University of Bern. Proposals for 2023 are most welcome!

6) Other applications: should be communicated to the president 10 days prior to the meeting.

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06.)	3	4
2017 (as of 17.07.)	10	4
2018 (as of 18.08.)	8	19*
2019 (as of 18.07.)	5	3
2020 (as of 17.08.)	10	13
2021 (as of 22.07.)	8	22

* in 2015, 2018 and 2021, a large number of SGK/SSCr members (18,19 and 22 resp.) have been excluded per decision of the Board because they were not paying the annual fees for more than 3 years, and/or could not be contacted.

Quorum for final decisions (Art.12, by-laws):
As of 22.07.2021, we have 184 records in our database.
They are grouped as:
- 8 of these are companies (or corporate members),
- 28 are “libraries” (incl. some “quasi-personal” members, from whom we don’t expect any fees, but to whom we are regularly sending our newsletters);
- 148 are personal members (full: 116, students: 28, honorary: 4)

I.e. for the quorum to be able to make decisions, we should have **10%** out of **152** corporate and personal members, i.e. at least **15** people.

Board Members:
see last page of this newsletter

Delegates

ECA:	A. Linden (Zurich)
IOCG:	E. Giannini (Geneva)
ScNat:	A. Neels (automatically assigned to the acting president)
Steering Comm. SNBL	G. Chapuis (Lausanne), R. Cerny (Geneva)
IUCR:	Anthony Linden (Zurich)
	Antonia Neels (Zurich)

Minutes of General Assembly 2020

Wednesday, September 9, 2020
Online meeting via ZOOM
10:00-11:40
Schweizerische Gesellschaft für Kristallographie

Agenda:

1) Determination of the quorum according to Art. 12/by-laws
2) Acceptance of the minutes of the General Assembly 2019, EPFL Sion
3) 2021/2022 Meeting and General Assembly: Decision on location/organizers (proposal 2022 in Bern, Simon Grabowsky)
4) Upcoming retirements from the Board and the election of new board members.
5) Reports
   a) Annual report
   b) Annual financial statement
   c) Budget for the next year
6) SNBL – updates on arrangements
7) Road-mapping for large scale facilities and SSPh
8) Travel grants and PhD prize for 2020/2021
9) Other motions of members

Minutes:

Formalities:

The General Assembly was chaired by Antonia Neels, President, and started at 10:00 h
The agenda has been published in the Newsletter 104 on 19. August 2020 (Art. 11)
The secretary Michael Wörle, ETH, was appointed as keeper of the minutes.

Ad 1.

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06.)	3	4
2017 (as of 17.07.)	10	4
2018 (as of 18.08.)	8	19*
2019 (as of 18.07.)	5	3
2020 (as of 17.08.)	10	13

* in 2015 and 2018, a large number of SGK/SSCr members (18 and 19, resp.) have been excluded per decision of the Board because they were not paying the annual fees for more than 3 years, and could not be contacted.

With 45 members being present at this assembly, the necessary quorum of 10% (17) is reached (Art. 12).
As of 18.07.2020, we have 199 records in our database.
They are grouped as:
- 8 of these are companies (or corporate members),
- 29 are “libraries” (incl. some “quasi-personal” members, from whom we don’t expect any fees, but to whom we are regularly sending our newsletters);
- 162 are personal members (full: 125, students: 33, honorary: 4)

10% out of 166 corporate and personal members, i.e. at least 17 people. Two corporate members present are Dubravka Sisak-Jung (Dectris AG), Eric Hovestreydt (ELDICO AG), (named according to Art. 14 of the bylaws).

Ad 2.
The minutes of the General Assembly 2019 on 04/09/2019 at EPFL Valais, reported in newsletter 104, have been approved unanimously, no abstentions.

Ad 3
The **Annual Meeting 2020**, originally planned to take place at the University Fribourg, had to be postponed because of restrictions connected to the Coronavirus-related situation. Accordingly, it is proposed that the **Annual Meeting 2021** will be organized by Katharina Fromm and Aurélien Crochet at the University Fribourg in September 2021. Further it is proposed that the **Annual Meeting 2022** will be organized by Simon Grabowsky at the University Bern in September 2022. **The proposals were accepted by 90% of the members, with 10% abstentions.**

Ad 4.
Two board members (Antonia Neels and Anthony Linden) will leave the board in 2021, since they will have served for the maximum of 9 years. The board of 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. The board appoints Simon Grabowsky, University Bern, as an extraordinary member for one year. An introduction

of Simon Grabowsky is given in the newsletter 104, page 19. It is desirable to find a representative of the protein crystallography community (proposal by Hans-Beat Bürgi) and/or from the neutron crystallography community (proposal by Radovan Cerny). AN said that the foreseen next 'Howard Flack Lecturer' with Ilme Schlichting, who is a structural biologist, presents a step into this direction: to get the biologist actively on board of the SSCr. The board will contact the respective groups and invite them to submit a proposal.

Ad 5 a).
Antonia Neels gives an overview on the conducted and planned activities of the SSCr in 2018-2021, as there was the Max-Perutz Symposium (15.04.2019), the SSCr Annual Meeting in Sion (04.09.2019) and the Howard Flack Lecture Series with Matt Rosseinsky (04-08.11.2019). Antonia Neels thanks all organizers of the Lecture Series, which was very successful. Prof. Matt Rosseinsky gave talks at CSEM Neuchâtel, University Fribourg, EPFL Lausanne and EMPA Dübendorf. Suggestions for 2021 are most welcome.
In 2019, 6 students were supported with travel grants, some of their reports were given in the newsletter 103.
The 2020 Powder Diffraction School at PSI (Sept. 2020) will take place live, although the number of participants is lower than usual due to travel restrictions. Because of international travelling restrictions, the Howard Flack Lecture Series 2020 has been postponed to 2021. Also scheduled for 2021 are the Annual Meeting in Fribourg (Sept. 2021), and the awarding of the PhD-prize of the SSCr.
SSCr members are very active in IUCr commissions such as the Commission on Journals, Aperiodic Crystals, Structural Chemistry and Magnetic Structures.

Dubravka Sisak-Jung gives an overview on the SSCr member survey, which was launched on 26.06.2020 in order to find out more on the expectations our members have. We had a satisfactory participation of about 30%. These data indicate that the SSCr members are mostly senior scientists, not involved in regular teaching, but highly involved in tutoring, organizing workshops and meetings. Predominantly used techniques are PXRD and single crystal diffraction, followed by neutron diffraction and electron microscopy. Instrumentation available in labs and in crystallography facilities reflects this distribution. The majority of respondents use large-scale facilities, predominantly SLS and SNBL, followed by SINQ and ILL.
The majority of respondents find the information on the instrumentation roadmap relevant, whereas only 11% of respondents are not aware of the roadmap.
The majority of respondents know about the current activities of the SSCr. The main expectation of the SSCr is to provide information about crystallography-related courses and teaching. Other expectations include: services of labs in Switzerland, online teaching, job opportunities, networking.
The board will reflect on these preliminary data at a later point.

Ad 5 b)
Budget report:
The treasurer *Enrico Giannini* gives the financial report for 2019.

Summary SGK Finances 2019

	CHF
Total 31.12.2018	**47’332.09**
UBS account	46’718.63
Cash on hand	533.25
Total 31.12.2019	**47’251.88**
Balance	**-80.21**

SGK Financial Report 2019

UBS Balance 31.12.2017	**30’798.60**
CS Balance 31.12.2017	**18’340.47**

Income:

Membership dues:	
Full members (various amounts due to debts)	
2x30 + 1x38 + 62x40 + 1x43.91 + 1x45.48 + 3x50 + 1x70 +19x80 + 1x84.50	
+ 1x100 + 3x120 + 1x150 + 1x220	5’276.41
Students 7x10 + 3x20 + 1x30	160.00
Companies 5x130 + 1x520	1170.00
Total membership	6606.41
Subsidy SCNaT (2018)	12’300.00
Interest	
	1.90

Total Income **18’908.31**

SGK Financial Report 2019

Expenses:

Membership dues to SCNat (163 members at 31.12.2019)	1'141.00
Travel costs for ECM delegates	1’000.00
Annual Meeting (PSI, Villigen)	3'000.00
Travel Grants	5’077.00
Howard Flack Lecture Series (Prof. Matthew Rosseinsky)	2’070.51
Support to the Zurich School of Crystallography	2’000.00
Satellite on neutron scattering at ECM32	1’500.00
Perutz symposium (collaboration with the SCS)	2’000.00
Association to ECA	200.51
Printing and publishing costs (newsletter)	830.15
Website	8.85
Bank expenses	160.50
Total Expenses	18‘988.52
Income – Expenses	-80.21

SGK Financial Report 2019

Cash on Hand - 2019:

Status 31.12.2018	**542.10**
Total Income	0.00
Total Expenses	8.85
Balance (Income – Expenses)	0.00
Starting Balance + Income – Expenses	533.25
Cash on Hand 31.12.2019	**533.25**

Revisorenbericht für die Jahresrechnung 2019 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS UBS 279-C0291110.0

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2019 bis 31. Dez. 2019. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2019 ist der Stand der Konten und der Kasse:

UBS	SFr.	46'718.63
Kasse	SFr.	533.25
Summe SGK	SFr.	**47'251.88**

Die Unterzeichneten beantragen von der Versammlung die Entlastung des Kassierers und der Revisoren für die geprüfte Periode.

Ort / Datum
Neuchâtel, 5. 2. 2020
Bern

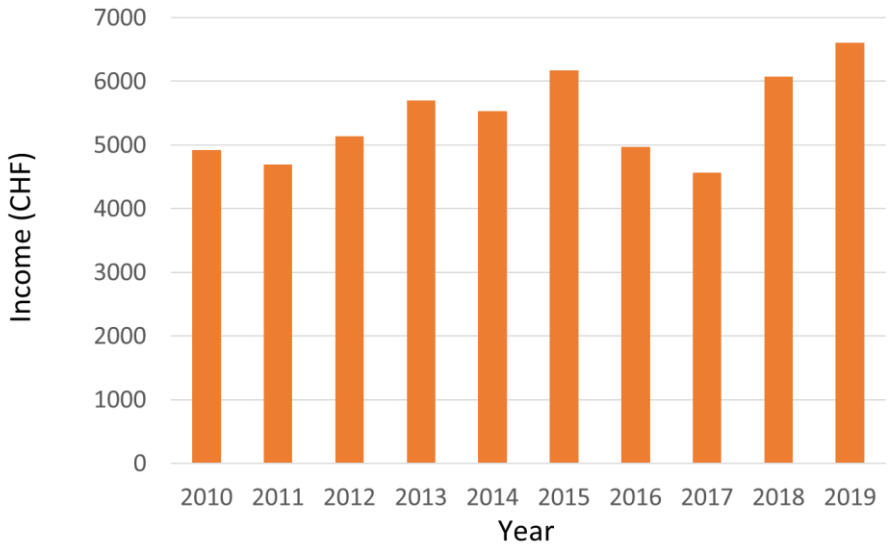
Unterschriften

B. Spingler
B. Spingler
(Universität Zürich)

K. Schenk
(EPF Lausanne)

- The budget 2019 has been approved by the auditors Kurt Schenk and Bernhard Spingler (Bern, 05.02.2020).

- *Enrico Giannini* presents an overview on the fluctuation of the membership dues. This year, many members paid their outstanding fees, which explains the fairly high income:



- Enrico Giannini reports on the SGK financial situation 2020: a “frozen “ year

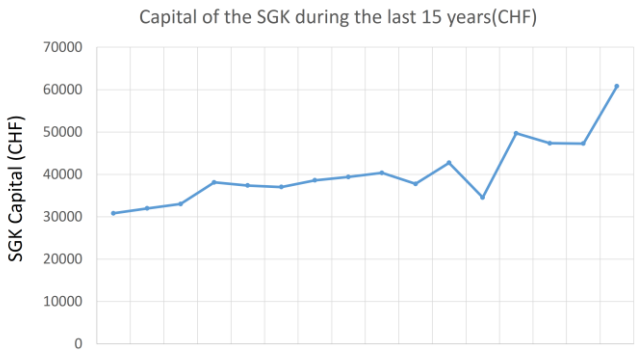
Credits:

Membership dues	5’048.00
SCNat contribution 2019	10’000.00
SCNat ECA membership	250.00
Total Income	**15‘298.00**

Debits:

Travel costs of delegates	409.36
ECA national membership dues 2019	190.38
Flack lecture series (2019)	337.68
Bank charges	46.00
PSI School	2'000.00*
IUCr delegates (IUCr25 in Prague)	2'000.00
SGK annual meeting (+ poster prize)	3'000.00
Howard Flack Crystallographic Lectures:	5'000.00
Travel grants for students	3’000.00
Membership dues to SANW	1'150.00
Publication costs	850.00
Total Expenses	**2‘983.42**

*Remark M. Wörle: The Powder School organized by the PSI was held on-line. The expenses were lower than CHF 2000.-. The exact amount has not been specified on the day of the General Assembly, but will be given in the next days.



The budget 2019 was approved with 85% of the votes, with 15% abstentions.

Ad 5 c)

SGK Budget proposal 2021

Credits:	
Membership dues	5'000.00
SCNat reimbursement for IUCr delegates (IUCr25 in Prague, Czech)	2'000.00
SCNat contribution for SGK annual meeting (including poster prize)	3'000.00
SCNat contribution for Zürich School	2'000.00
SCNat PhD / master students travel grants	4'000.00
SCNat Crystallographic Lectures: Howard Flack Series	3'000.00
SCNat ECA membership	250.00
Publication costs	500.00
Total Income	**19'750.00**
Debits:	
Membership dues to SCNat	1'150.00
Annual meeting + poster prize	3'000.00
Travel Grants for Young Scientists	6'000.00
PhD thesis prize	2'000.00
SGK support for Zürich School	2'000.00
Crystallographic Lectures: Howard Flack Series	4'000.00
IUCr delegates (IUCr25, Prague, Czech)	2'000.00
Sponsoring and event advertisement (posters, flyers, webpage)	2'000.00
ECA national membership dues 2019	250.00
Publication costs	1'000.00
Bank charges	200.00
Total Expenses	**23'600.00**
Income – Expenses	**- 3'850.00**

Some remarks of Enrico Giannini: In 2021 we will be able to fund 10 travel grants for students

The budget 2021 was approved with 81% of the votes, with 19% abstentions.

Ad 6)

Radovan Cerny gives a report on the news concerning the financing of the SNBL beamline (Grenoble) in the future. The PSI, the actual contractual partner of the SNX (The Swiss members of the SNX are of Radovan Cerny (Uni Geneva), Wendy Queen (EPFL) and Paula Abdala (ETH)), has decided not to renew the SNX agreement with Norway beyond 2020. Recently, EPFL agreed to act as contracting partner for the period 2021-2024, which is a major success. However, financing has to be taken by the users in the period 2021-2024, who have to pay 2.68 kFr. per shift. In the case of users from ETHZ and EPFL, both institutions will pay for 2/3 of the amount. Users from other universities have to negotiate with their institutions for support, but will in any case be billed by EPFL for the full shift costs. These costs do not apply if the user successfully applies for beam time through the ESRF proposal system. Users are encouraged to submit proposals (the next deadline is 10 October 2020). The following table gives the prospective financial situation for three 4-year-periods:

2017 – 2020	Swiss contribution (50% of the total budget) 820 – 865 kEUR, paid by SERI
	Contracting partner PSI
2021 – 2024	Swiss contribution (50% of the total budget) 770 kEUR, paid by Swiss users
	(~2.68 kEUR / shift)
	Contracting partner EPFL
2025 - 2028	SNBL part of the Swiss Roadmap for the research infrastructure as an operando center
	Swiss contribution paid by SERI

Radovan Cerny also reports the new plans to implement a **Center for Operando Synchrotron Studies:**
Research Infrastructure for *operando* synchrotron based real time studies from the atomic to nanometer and electronic structures, by combining a wide range of X-ray spectroscopy and diffraction techniques under operando conditions, complimented by operando IR/Raman and UV-VIS studies.
Aims:

- Provide rapid access to dedicated synchrotron instruments
- Provide expert user support, big data management and data analysis tools
- Provide both: high throughput (east hub) and tailor made (west hub) *operando* synchrotron tools

Community: Chemistry/Physics/Materials Science/Geoscience/Biology
Location: east Hub at SLS-PSI, west Hub at SNBL-ESRF (Grenoble/France)
Investment Plans: Development of: multi-technique experimental technology, operando cells, data analysis software and data platform, transferable between hubs
Personal: 9 FTE at the East Hub, 4.5 FTE at the West Hub for support from experiment to data analysis and management.
Budget (Phase 1 – 2025-2028): 13.2 MCHF

Ad 7)

Antonia Neels presents the SCNat Roadmap 2025-2028 for the scientific research infrastructures. Details can be found on the website of the SCNAT: On a mandate of the Confederation, SCNAT develops roadmaps for scientific research infrastructures. These will form the basis for the Swiss Roadmap for Research Infrastructures (RIs). This roadmap of national and international RIs of interest for Switzerland is used to decide which large research facilities deserve federal support. On request by the SERI, SCNAT develops discipline-specific roadmaps for the natural sciences. These point out which research infrastructures will be necessary in the future and prioritise them from a scientific point of view. The SERI will evaluate the roadmaps for the various fields together with other actors and will decide which research infrastructures are to be included in the 2023 Roadmap and then, possibly, in the ERI Dispatch 2025–2028. https://naturalsciences.ch/organisations/scnat/for_a_solid_science/networks_and_infrastructures/research_infrastructures
The time schedule foresees an elaboration of the discipline specific roadmaps and a submission to SERI in early 2021. The Swiss Society for Photon Science (SSPh) has been given the task to create a road map on photon science. The following people are involved, covering the different disciplines:

Urs Staub (PSI, Microscopy and Magnetism)
Claude Monney (UniFR, ultrafast spectroscopies: photoemission spectroscopy and resonant inelastic x-ray scattering)
Marco Stampanoni (PSI, X-ray imaging)
Dimitrios Fotiadis (Biozentrum, Uni Basel, Structural Biology)
Jean-Marc Jeckelmann (UniBe, Biochemistry and Molecular Medicine)
Wendy Queen (EPFL, Functional Inorganic Materials)
Antonia Neels (SSCr, Empa, Materials Science)

Antonia Neels has reached out to the crystallographic and synchrotron user community:

- SSCr / SGK questionnaire: sent out in June 2020
- E-mail sent out to the SLS (PSI) and SNBL (ESRF) user community
- Proposal to create a ”Center for operando synchrotron studies”: from Chemistry roadmap community

The feedback from the user community is/will be integrated into the final document.
An important on-line ZOOM meeting for the synchrotron users titled “
“Synchrotron tools for the chemistry/ materials science community beyond 2024: quo vadis?” will take place on 16. Sept. 2020.

The SSPh (http://swissphotonscience.ch/) has been founded in 2019 for representing the scientists active in the fields of optics, photonics and spectroscopy towards official bodies, such as the Swiss Academy of Sciences and SERI. *Anthony Linden* gives an overview on the SSPh. Since the SSPh was contracted by SCNat for the development of the Roadmap and also SERI exchanges regularly information with SSPh, the SGK should decide how to make sure that the diffraction community will be represented and heard, too. Therefore, the SGK encourages its members to become individual members of the SSPh. In addition, the SGK should become an institutional member. The board will get in will contact with the president of the SSPh and propose to install a 6th seat for the SGK in the board of the SSPh or nominating a candidate for the board at the next election (proposal Anthony Linden). SCNat will be made aware that the diffraction community is not yet fairly represented within the current setup.
Ad 8) (responsibility assignment in an upcoming board meeting).

Antonia Neels reminds the members of the travel grants in 2020/2021. 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. Financial support can also be granted to retired SSCr members

In 2021 there will be again a Swiss Society for Crystallography PhD prize award for students who have earned the title between March 31st 2019 and March 31st 2021. The application for the prize should be submitted before 31st May 2021 by the student himself or by the thesis supervisor. The application should be sent to the secretary of the Swiss Society of Crystallography (info@sgk-sscr.ch). An corresponding announcement will be published in the upcoming newsletter 105 (March 2021).

Hans-Beat Bürgi and Nicola Casati proposed to offer some time slots for talks on protein crystallography at our Annual Meeting (see also Ad 4, concerning new board members). The board will reach out to relevant people/groups active in the protein crystallography community (Basel Biocenter, PSI, Bern) in order to encourage them to join SSCr. This will strengthen the SSCr's position. In addition, inviting Ilme Schlichting as speaker in the Howard Flack Lecture Series 2021 will be a good opportunity to strengthen the contacts with the protein crystallography community (responsibility assignment in an upcoming board meeting).

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Meeting ends at 11:40

Minutes written by the Secretary
Michael Wörle, 09.09.2020

Approved by the President
Antonia Neels

Swiss Society for Crystallography PhD prize

The **winner 2021** will be announced at the beginning of August on the following web-site:

https://sgk-sscr.ch/

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

13.9.2021, 4-5pm

Prof. Michael Hothorn,

‘Plant signal transduction cascades – from atoms to phenotypes and back’

UNIVERSITÉ DE GENÈVE

11.10.2021, 4-5pm
Prof. Jan Pieter Abrahams

‘Catalytic cycling of human mitochondrial Lon protease’

University of Basel

15.11.2021, 4-5pm
Prof. Amedeo Caflisch

‘Protein structure-based drug design’

University of Zurich[UZH]

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.

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.

Meetings, Conferences, Workshops, Schools, Courses

IUCR XXV

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/

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	15.01.2022	https://www.esrf.fr/home/UsersAndScience/latest-news-for-users/content-news/esrf-news-list/next-deadlines-for-proposal-submission.html
short term proposals (standard)	13.09.2021	
Macromolecular BAG Proposal	13.09.2021	
ILL: Institut Laue Langevin		
All instruments	tba	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 Oak Ridge	22.09.2021	neutrons.ornl.gov

Calendar of forthcoming meetings

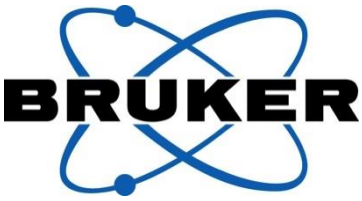
(Please mail the missing information on meetings of interest to woerle@inorg.chem.ethz.ch)

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/	Abstracts 16.05.2022
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://www.ecm33.fr/	Start Abstract submission 31.01.2022
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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SGK/SSCr Newsletter (ISSN 1662-5358, online version: ISSN 1662-534X)

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IBAN: CH39 0027 9279 C029 1110 0
BIC: UBSWCHZH80A
BLZ: 279

Printing and

Mailing:

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

The newsletter of SGK/SSCr is published 2-4 times a year in a circulation of 250. Contributions are welcome at any time, as well as illustrations for the cover. Articles in English, German or French may be submitted. Please send all interesting material directly to the editor.
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