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No. 110
August 2023

"Newest Developments in Crystallography and related topics"

In this issue: Program of the SSCr Annual Meeting and General Assembly 2023

On the Cover:
Invitation to the SSCr Annual Meeting and General Assembly 2023 in Zurich

The President's Page

Dear members,

You are most likely enjoying the summer break with your beloved ones, some of you surely while preparing for IUCr in Melbourne. From my side I send you my summer greetings from Brittany, from where I am writing this message to you in preparation for our second newsletter this year.

The approaching IUCr is exciting for our board this year in a number of ways, since we are organizing a satellite workshop which takes place on August 21st and is booked out completely. Congratulations to Dubravka who has been taking the lead on this initiative, with Paula's usual indispensable support.

Times will remain busy for the SSCr and its board, with the co-organization of the Erice school in 2024, chairing of the CECAM meeting in Lausanne in 2025, the outstanding EPDIC19 bid which we will focus on end of this year, and, importantly, the second edition of our own topical workshop which we introduced this year with SAXS and for which the interest has been overwhelming with 62 registrations. Next year's topic has already been decided upon and will deal with total scattering. The stage for this will be set with November's Flack Lectures. Our Flack Lecturer Simon Billinge will be visiting Sion, Bern, Basel, at Dectris, PSI and in Zürich. You will find an abstract and announcement in this newsletter, and more information on our website and social media very soon.

I am happy and grateful to Bernhard Spingler that we have managed to bring the annual meeting to UZH this year on Friday, which Bernhard is hosting on September 8th, running the general theme "Newest Developments in Crystallography". As far as I am aware this is the first time we have a stand-alone SSCr event at UZH; exciting! Likewise, the SSCr is very fortunate that next year's annual meeting in 2024 will also come to a location we have not yet been to before. It is nice to see that the board's efforts throughout the past years are being rewarded. New memberships are picking up again as well, which is also reflected in the number of travel grants awarded this year. Plus, two excellent candidates had a head-on-head race for this year's PhD prize. I look forward to the prize lecture during the annual meeting in Zürich.

At the same time, we say good bye to Olha, who will retire from the board this year. We thank you, Olha, for your constructive efforts in the past and hope to see much of you in the future. The General Assembly will be voting on new board members in Zürich.

I would like to point out that the Department of Materials of ETHZ is on a run, with two SSCr members receiving awards for outstanding achievements relating to crystallography. Congratulations from all of us! With the Will-Kleber Commemorative Coin our colleague Thomas Weber receives the award for his methodological work on the study of disordered crystals using diffuse X-ray scattering. Still related to diffuse scattering, Arkadiy Simonov is awarded the W. H. and W. L. Bragg Prize for outstanding early-career crystallographers for his development of the three-dimensional difference pair distribution function (3D-∆PDF) approach and its transformative effect on the field of materials. Don’t miss Arkadiy’s lecture in Melbourne.

In this edition of the newsletter you will find two topical contributions on pair distribution function analysis by Bruker and Malvern Panalytical, which nicely show what can be done in the lab nowadays. Please feel free to do likewise and submit your own contributions. The SSCr is the Forum for Swiss crystallographers and materials scientists in a small but busy and focused society.

I wish you a successful IUCr and hope to see you soon in Zürich,

Pascal Schouwink

The SSCr Annual meeting 2023

University of Zurich UZH

"Newest Developments in Crystallography and related topics"

Invited Speakers

Prof. Raimund Dutzler, University of Zurich
Dr. Brian Pauw, Bundesanstalt für Materialforschung und -prüfung (BAM)
Prof. Clemens Richert, University of Stuttgart

Information

Friday, September 8th, 2023
8:30-17:30

University of Zurich
Irchel campus
Lecture Hall 35 F 32
Winterthurerstrasse 190 8057 Zürich
Trams 9 or 10 till tram stop “Irchel”.

The traditional dinner will be held on September 7, 6:30 p.m. at the Wild West Steakhouse TEXAS.
The restaurant is in the Irchel park between the tram stop “Irchel” and the Irchel campus.

ema.uzh.ch/RG7RK

Organizer:
Prof. Dr. Bernhard Spingler
Department of Chemistry University of Zurich

Scientific Programme

Annual Meeting Swiss Society for Crystallography

8 September 2023

09:00		Registration & coffee
09:25	Bernhard Spingler	Welcome address
	Chair: Antonia Neels	**Materials and minerals I**
09:30 – 10:00	Invited speaker: Brian Pauw	Glimpses of the future: advancing X-ray scattering in an automated materials research laboratory
10:00 – 10:12	Yevheniia Kholina	Hidden phase transition upon dehydration of Prussian Blue analogues (PBAs)
10:12 – 10:24	Yaser Balmohammadi	Evaluating the nature of arsenic-involving bonds / interactions related to piezoelectric properties using quantum crystallography and complementary bonding analysis
10:24 – 10:36	Bruno F.B. Silva	Microfluidics with in-situ SAXS for time-resolved studies of liquid crystal dissolution
10:36 – 11:05		Coffee break, **posters** and sponsors
	Chair: Paula Abdala	**Materials and minerals II**
11:05 – 11:17	Thomas Weber	Novel diffraction strategies to unravel hidden order in ferroelectric thin films
11:17 – 11:29	Rohan Pokratath	Colloidal Synthesis of Zirconia Nanocrystals: Precursor Conversion to Crystallization
11:29 – 11:41	Annelies Landuyt	Boosting the CO_2 Uptake of MgO-based Sorbents with Na_2CO_3 as Nucleation Seeds: Mechanistic Insight via Time-Resolved XRD
11:41 – 11:53	Przemyslaw Rzepka	Locating Al in zeolite frameworks by exploiting anoma-lous X-ray powder diffraction at the Al absorption edge
11:53 – 12:05	Sabrina L. J. Thomä	Pair distribution function (PDF) analysis – from nanoparticle dispersions to bulk metallic glasses
12:05 – 12:17	Diana Piankova	Electron PDF - a tool to study local order in poorly crystalline-, nano-, and amorphous materials
12:17 – 14:15		Lunch, **posters** and sponsors
13:15 – 14:15	for SSCr members	**SSCr Annual General Assembly**
14:15 – 15:15	Chair: Peer Mittl	**Structural biology**
14:15 – 14:45	Invited speaker: Raimund Dutzler	Structural basis for ion selectivity in the SLC11/NRAMP family of transition metal ion transporters
14:45 – 14:57	Mariia Savchenko	Protein crystals as a template for in situ formation of magnetite nanoparticles
14:57 – 15:09	Peer Mittl	Host lattice display: a method for the analysis of biomolecules
15:09 – 15:40		Coffee break, **posters** and sponsors
15:40 – 17:19	Chair: Alessandro Prescimone	**Chemical crystallography**
15:40 – 16:15	PhD SSCr Price lauréate	
16:15 – 16:27	Adriana Torres-Mansilla	Heterogeneous Nucleation on The Eggshell Membrane: Sustainable Development of Biomaterials for Bone Regeneration
16:27 – 16:39	Tobias Stürzer	Bridging the gap between Electron and X-ray Diffraction
16:40 – 17:20	Invited speaker: Clemens Richert	Tetraaryladamantanes as Crystallization Chaperones for Liquids
17:20		**Poster prize, concluding remarks**

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SSCr Annual Meeting 2023: Abstracts for Talks

Glimpses of the future: advancing X-ray scattering in an automated materials research laboratory

Brian R. Pauw, Glen J. Smales, Ingo Bressler, Sofya Laskina, Aaron Chambers

Bundesanstalt für Materialforschung und -Prüfung, Unter den Eichen 87, 12205 Berlin, Germany

In our (dramatically understaffed) X-ray scattering laboratory, developing a systematic, holistic methodology[1] let us provide scattering and diffraction information for more than 2100 samples for 200+ projects led by 120+ collaborators. Combined with automated data correction pipelines, and our analysis and simulation software, this led to more than 40 papers[2] in the last 5 years with just over 2 full-time staff members.

This year, our new, modular synthesis platform has made more than 1000 additional samples for us to analyse and catalogue. By virtue of the automation, the synthesis of these samples is automatically documented in excruciating detail, preparing them for upload and exploitation in large-scale materials databases. Having developed these proof-of-concepts, we find that materials research itself is changed dramatically by automating dull tasks in a laboratory.

This talk is intended to spark ideas and invite collaborations by providing an overview of: 1) the current improvements in our wide-range X-ray scattering laboratory methodology, 2) Introduce some of our open-source analysis and simulation software, touching on scattering, diffraction and PDF, and 3) introducing our open, modular robotic platform for systematic sample preparation. Finally, the remaining bottlenecks and points of attention across all three are highlighted.

Figure 1: the MOUSE X-ray scattering instrument.

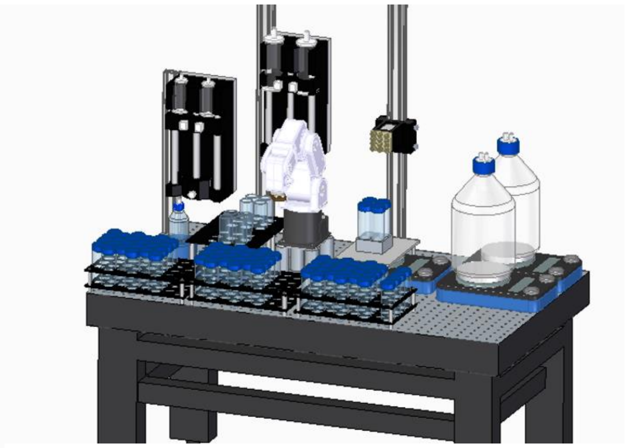

Figure 2: the automated, modular synthesis platform RoWaN.

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(2) https://scholar.google.com/citations?user=YKnAFTcAAAAJ

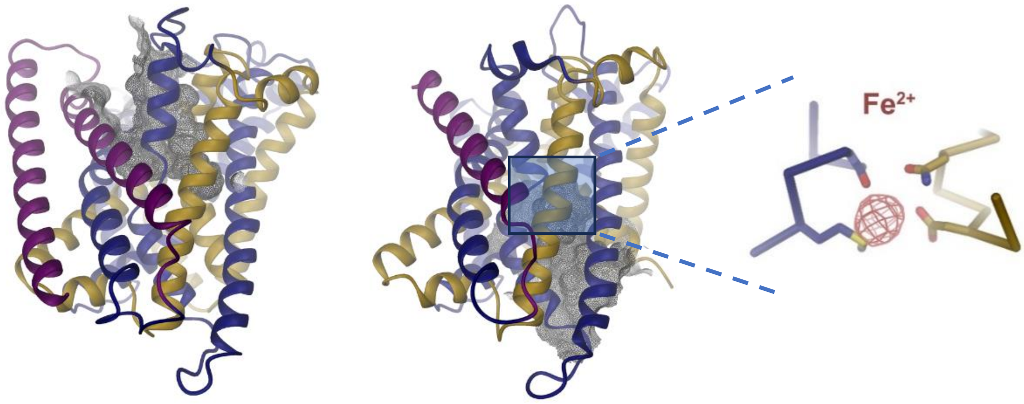
Talk

Structural basis for ion selectivity in the SLC11/NRAMP family of transition metal ion transporters

Raimund Dutzler

Department of Biochemistry, University of Zurich, CH 8057 Zurich, dutzler@bioc.uzh.ch

Members of the ubiquitous SLC11/NRAMP family catalyze the uptake of divalent transition metal ions into cells. They have evolved to efficiently select these trace elements from a large pool of Ca^{2+} and Mg^{2+}, which are both orders of magnitude more abundant, and to concentrate them in the cytoplasm aided by the cotransport of H^+ serving as energy source. By employing an interdisciplinary approach combining X-ray crystallography, cryo-electron microscopy and various binding and transport assays, my group has over the years defined the mechanistic basis for the unique ion selectivity of this family[1-3] and of close homologs with altered substrate preference[4,5].



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Talk

Tetraaryladamantanes as Crystallization Chaperones for Liquids

Clemens Richert, Tim Berking, Wolfgang Frey

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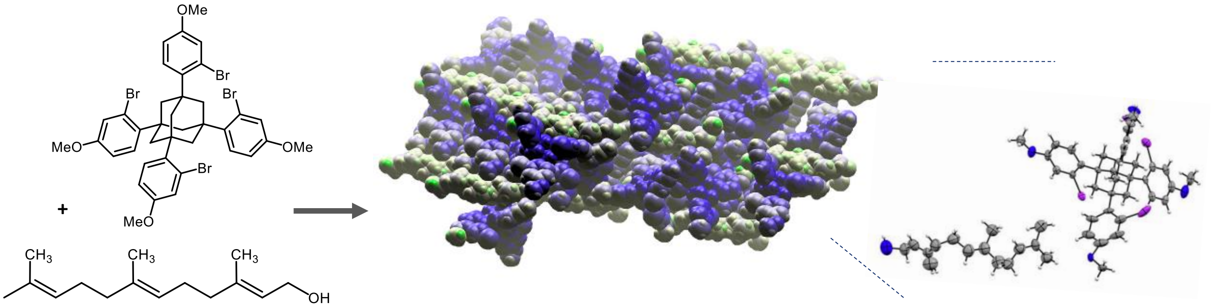
Obtaining a crystal structure of compounds that are liquids at room temperature is a challenge. Low temperature methods exist,[1] but they require instrumental effort and considerable experimental skill. Alternatively, crystalline sponges[2] or hydrogen-bonded frameworks[3] may be employed. We have recently observed that certain tetraaryladamantane ethers readily crystallize as solvates after having been briefly heated with the liquid of interest.[4] This method can be used to determine the absolute configuration of analytes by X-ray crystallography.[5]



In the presentation, the molecular basis for the chaperone effect of tetraaryladamantanes will be discussed.

Financial support by DFG, grant No. RI-1063/17-1, is gratefully acknowledged

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Talk (12 min)

Hidden phase transition upon dehydration of Prussian Blue analogues (PBAs)

Yevheniia Kholina, Arkadiy Simonov

Laboratory for Disordered Materials, Department of Materials, ETH Zürich, CH 8093,
yevheniia.kholina@mat.ethz.ch

Prussian blue analogues (PBAs) are a diverse family of transition metal cyanide materials with chemical formula $M[M'(CN)_6]_{1-x}\square_y\cdot nH_2O$, which we abbreviate here as M[M’] (M and M’=transition metal ions, □=vacancy). These materials are known for their highly connected porous network, enabled by structural vacancies of M’(CN)6 with sufficiently large channels to transport or store small molecules and ions. Currently these systems are actively investigated for application as hydrogen storage media, humidity sensors, and alkali ion sieves.

One step which is often overlooked in the research is drying. PBAs are typically grown from water solutions and water has to be removed by heating the sample either in vacuum or in dry atmosphere. Since drying doesn’t change the average structure, it is generally assumed that this step doesn’t alter the porous network of PBAs. We demonstrate that dehydration step in fact causes a hidden phase transition that involves irreversible rearrangements of vacancies. Such rearrangements modify the pore-network characteristic, like fraction of accessible volume and conductance of matter through the channels. We collect diffuse scattering from Mn[Co] single crystals and use 3D-ΔPDF analysis to characterize their local structure and monitor any structural changes upon water removal. We also demonstrate that same material dehydrated at slightly different conditions shows different performance, drawing a link between a local structure and materials properties.

Reference

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Talk (12 min)

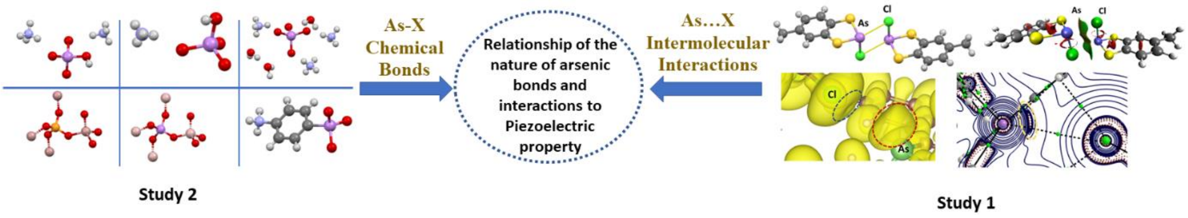
Evaluating the nature of arsenic-involving bonds/interactions related to piezoelectric properties using quantum crystallography and complementary bonding analysis

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

University of Bern, Department of Chemistry, Biochemistry and Pharmaceutical Sciences, Freiestrasse 3, 3012 Bern, Switzerland, simon.grabowsky@unibe.ch

Elemental arsenic and its compounds have many applications in bio/materials science, but the nature of arsenic bonds/interactions is not clear yet. $GaAsO_4$ is a piezoelectric material. The mainstay of piezoelectricity is the nature and geometric arrangement of the polar intra/intermolecular interactions. To understand the relationship between piezoelectric property and the bonding situation in arsenic materials, we need to understand first the behaviour of arsenic in chemical interactions/bonds. To this end, we studied two different structure sets of arsenic compounds as model structures to compare with piezoelectric $GaAsO_4$.

In the first study, to understand the nature of arsenic-involving intermolecular interactions and the effect of oxidation state, 77 crystal structures selected that include both oxidation states of arsenic (III/V).[1] In the second study, a series of arsenic compounds with As-O bond/interactions were examined. As_3O_6, $AsO_4(NH_4)_3(H_2O)_3$, $HAsO_4(NH_4)_2$, $C_6H_8NAsO_3$, $C_6H_{10}N_3O.AsH_3O.AsH_2O_4$, and $GaAsO_4$ are our compounds. Figure bellow shows a schematic representation of our study.



For the first study, the properties and nature of arsenic interactions were characterized by different bond descriptors (complementary bonding analysis).[2] Our results show that As(III) species act ambivalently in their interactions as Lewis acids or bases due to a lone pair, forming halogen, pnicogen, and chalcogen bonds, unlike As(V) which is only a Lewis acid.[1]

Next, for our high-resolution home-sources and synchrotron XRD data, Hirshfeld atom refinements (HAR) along with x-ray constrained wave function fitting (XCW), and DFT calculation were performed. QTAIM results for model demonstrate that As-O bonds have a positive value of electron density Laplacian which categorized them as a closed-shell interaction. Therefore, the As-O bond is likely to be charge-separated not a hypervalent bond. ELI-D analysis also shows both covalent and ionic characteristics of the As-O bond depending on the chemical environment and the partner of arsenic in that chemical bond. This knowledge assists us to understand the relationship between the nature of the chemical bonds/interactions and the piezoelectric property.

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Talk (12 min)

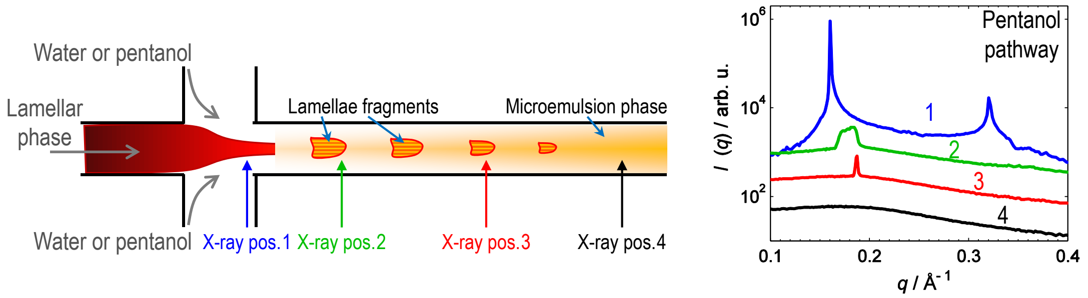
Microfluidics with in-situ SAXS for time-resolved studies of liquid crystal dissolution

Bruno F.B. Silva

Center for X-ray Analytics, Laboratory for Biointerfaces and Laboratory for Biomimetic Membranes and Textiles, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen 9014, Switzerland, *bruno.silva@empa.ch*

Microfluidic devices combined with in-situ small-angle X-ray scattering (SAXS) constitute a promising method for studying soft matter under non-equilibrium conditions[1,2]. These devices enable precise control and reproducibility over key parameters such as mixing rates, shear rates, concentration gradients, and confinement when fluids flow in micron-sized channels, enabling novel experiments[3].

In this study, we probe the dissolution of a lamellar liquid crystalline phase into water- and oil-rich microemulsions by mixing an SDS-based lamellar phase with either water or pentanol in a crossed microchannel configuration (figure)[4]. Through careful adjustment of the flow rates, we accurately control the final composition and dissolution rate, allowing us to explore the transition across different time scales. In-situ SAXS provides real-time monitoring of the structural evolution. The main findings show that the lamellar to o/w microemulsion transition (by mixing with water) occurs through a gradual stripping down of bilayers from the lamellar phase, whereas the lamellar to w/o reverse microemulsion transition (by mixing with pentanol) involves the formation of an intermediate lamellar phase with a *d* spacing gradient across the droplet.



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Talk (12 min)

Novel diffraction strategies to unravel hidden order in ferroelectric thin films

Joohee Bang[1], Nives Strkalj[2], Martin Sarott[1], Morgan Trassin[1], Thomas Weber[1]

[1] Department of Materials, ETH Zurich, Switzerland
[2] Department of Materials Science and Metallurgy, Cambridge University, United Kingdom

Ferroelectric thin films attract great attention for their rich applications in energy-efficient electronic devices with relevant physical properties such as high dielectric constants, electrically switchable polarization, and nonlinear piezoelectric effects. Previous approaches to characterizing the complex local atomic structures and corresponding polarization states of these materials have been largely limited to electron microscopic methods, which provide essentially two-dimensional information about small subvolumes of the sample, while X-ray methods were mostly used for microstructural characterization (mosaicity, epitaxial growth, domain size, etc.)[1]. With both approaches, the characterization of the local structure is incomplete. In this contribution, we show a comprehensive X-ray investigation of the reciprocal space of complex thin film multilayer structures. Stacks of various $[(PbTiO_3)_m|(SrTiO_3)_n]_p$ multilayers (*m*, *n* = 3, 5, 7; *p* = 10, 12) were eptitactically grown on $SrTiO_3$ substrates and investigated using gracing incidence single crystal diffraction methods. Experiments were performed at low and high temperatures at the beamlines SNBL@ESRF with X-rays of conventional wavelength and moderate incidence angle of ~2°, and P07@DESY with high X-ray energy and ultra-small incidence angle of ~0.03°. The local structure is investigated using the 3D-ΔPDF method[2]. To the best of our knowledge, this is the first time such a comprehensive study of local order in thin films has been performed. Examples of the variety of diffraction information accessible with our method are shown in Fig. 1.

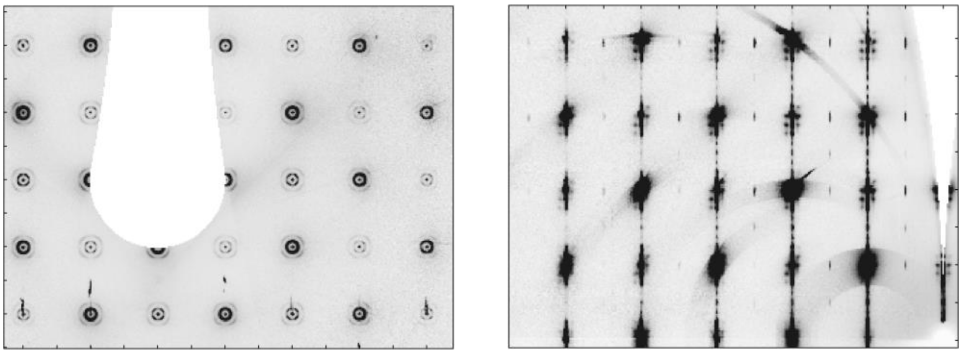

Fig 1: Left: *hk*6.82 section of $(PbTiO_3)_5|(SrTiO_3)_5$, Right: *h0l* of $(PbTiO_3)_3|(SrTiO_3)_5$

We thank the Swiss National Science Foundation for financial support.

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Talk (12 min)

Colloidal Synthesis of Zirconia Nanocrystals: Precursor Conversion to Crystallization

Rohan Pokratath,[1]* Lermusiaux Laurent,[2] Stefano Checchia,[3] Jikson Pulparayil Mathew,[1] Simon J. L. Billinge,[5] Benjamin Abécassis,[2] Kirsten M. Ø. Jensen,[4] Jonathan De Roo[1]

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[2] Univ Lyon, ENS de Lyon, CNRS, Université Claude Bernard Lyon1, Laboratoire de Chimie, Lyon, France

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[4] Department of Chemistry, University of Copenhagen, Universitetsparken 5, Copenhagen Ø 2100, Denmark

[5] Applied Physics and Applied Mathematics Department, Columbia University, New York, NY 10027, USA

One can nowadays readily generate monodispersed colloidal nanocrystals, but a retrosynthetic analysis is still not possible since the underlying mechanism is often poorly understood. A genuine mechanistic model can provide fundamental scientific interpretation to the chemical system and initiate evolution in synthetic strategies. In this work, we unknot the formation mechanism during the surfactant-assisted non-aqueous synthesis of zirconia nanocrystals. First, we identify the active precursor species in the reaction mixture using a powerful combination of nuclear magnetic resonance (NMR) spectroscopy, *in situ* X-ray pair distribution function (PDF) analysis, gas chromatography (GC-FID), and density functional theory (DFT) calculations.[1] After elucidating the precursor chemistry, we turned to nucleation and growth mechanism. X-ray scattering techniques were chosen for investigating the atomic-scale structural evolution and particle concentration estimation. We find that initially, many amorphous particles are formed. Over time, the total particle concentration decreases while the amorphous particles recrystallize into ZrO_2 nanocrystals.[2] The non-classical nucleation is likely related to the precursor decomposition rate that is an order of magnitude higher than the observed crystallization rate. A thorough understanding of the crystal structure of the nanoparticles will serve to formulate a structure-function correlation. The combined outcome of the precursor chemistry and the crystal growth will enable the rational design and synthesis of complex oxide nanocrystals which will serve as valuable building blocks in material science.

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Talk (12 min)

Boosting the CO_2 Uptake of MgO-based Sorbents with Na_2CO_3 as Nucleation Seeds: Mechanistic Insight via Time-Resolved XRD

Annelies Landuyt*, Ilia Kochetygov**, Maximilian Krödel*, Paula M. Abdala*, Wendy L. Queen**, Christoph R. Müller*

* Laboratory of Energy Science and Engineering, ETH Zürich, CH 8092 Zürich

** Institute of Chemical Sciences and Engineering, EPFL Sion, CH 1951 Sion

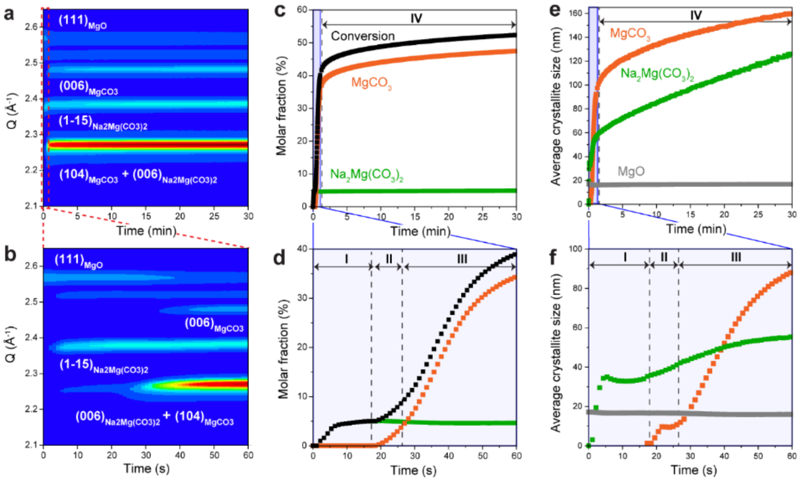

Figure 1. (a) 2D contour plot of the XRD data during the carbonation of ($Na_2CO_3/NaNO_3$)-promoted MgO (315 °C, CO_2). (c) The molar fractions of $MgCO_3$ and $Na_2Mg(CO_3)_2$ and the MgO conversion as a function of time. (e) The average crystallite size of $MgCO_3$, $Na_2Mg(CO_3)_2$ and MgO as a function of time; (b,d,f) A zoom in on the first 60 s.

To reach net zero CO_2 emissions and mitigate global warming, CO_2 capture is a key technology. Therefore, there is an urgent need to develop functional materials that can capture and release CO_2 on demand. Solid oxide materials such as MgO are earth-abundant and constitute a promising family of materials for CO_2 capture, utilization, and storage (CCUS). [1] However, MgO-based sorbents suffer from slow carbonation kinetics. The addition of molten salts, such as $NaNO_3$ can promote $MgCO_3$ formation by dissolving $[Mg^{2+}\cdots CO_3^{2-}]$ ionic pairs. [2,3] Here, we engineer an effective CO_2 sorbent, by co-promoting MgO with $NaNO_3$ and Na_2CO_3. In-situ synchrotron XRD measurements show that Na_2CO_3 first transforms into $Na_2Mg(CO_3)_2$ that acts as a nucleation site (seed) for $MgCO_3$ growth, boosting the CO_2 uptake. Furthermore, the nucleation and growth kinetics extracted from the in-situ XRD data in combination with insights from electron-based techniques allowed a mechanistic understanding of the role of $Na_2Mg(CO_3)_2$. The rate-limiting step for the CO_2-uptake of MgO is the nucleation of $MgCO_3$ and the presence of $Na_2Mg(CO_3)_2$ leads to fast $MgCO_3$ nucleation, resolving the poor kinetic performance of MgO sorbents. We believe that the insight obtained here using in situ time resolved studies can guide the rational advancement of CO_2 sorbents.

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Talk (12 min)

Locating aluminum in zeolite frameworks by exploiting anomalous X-ray powder diffraction at the Al absorption edge

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An active site within zeolite structures consists of a pair of negatively charged aluminum atom substituting silicon in the zeolite framework, along with an extra-framework cation. When the cation is a proton, the zeolite stays active in Brønsted-acid catalyzed reactions. However, direct observation of protons via X-ray methods is challenging due to their low mass, and thus, the positions of aluminum in the framework solely determine the accessibility and geometry of the active sites.

Numerous techniques have been applied to locate aluminum within zeolite catalysts, but they have provided only partial information, making it difficult to identify which T sites in the zeolite framework are occupied by aluminum. Given that most zeolites contain low aluminum content (typical zeolite catalysts have Si:Al ratios larger than 5), and aluminum's scattering power is similar to silicon, this task becomes very challenging.

To address this challenge, we have developed an innovative approach that exploits the diffraction technique at the Al X-ray absorption edge.[1] At X-ray energies far from the edge, the X-ray atomic scattering factor, $f = f_0 + f' + if''$, is primarily a function of the number of electrons in the element (f_0, e.g., 13 for Al and 14 for Si). As the energy approaches an element's edge, the f' and f'' contributions become significant, leading to changes in the scattering power of that element. At the Al absorption edge (1.56 keV), the scattered signal for aluminum decreases while that for silicon remains unchanged (Figure 1). This difference affects the intensities of the Bragg reflections and allows the aluminum positions in the structure to be determined.

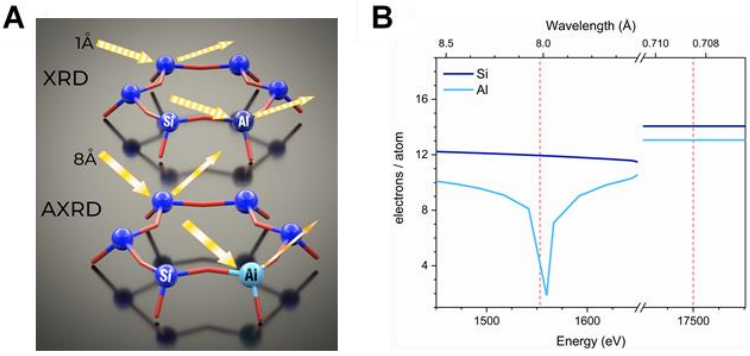

Figure 1. A: Visualization of the anomalous X-ray diffraction at the Al absorption edge, where the signal for Al is strongly reduced. **B:** X-ray scattering factors $f_0 + f'$ for Si and Al.

Two **FER**-type zeolites with identical compositions ($|H_{2.2}|[Si_{33.8}Al_{2.2}O_{72}]$), but different catalytic activities, were investigated. They were synthesized under conditions that aimed to alternate the Al distribution. The materials appeared to be ideal candidates to test the viability of the method and its detection limits (Si:Al ratios ca. 15). One sample was more active and selective in the isomerization of n-butene to i-butene than the other, but also deactivated faster.[2] The aluminum can be located at the four different T sites in the **FER**-type structure. One sample exhibited an even distribution, while the other showed aluminum concentrated on the T1 and T3 sites. More aluminum located respectively on the T2 site led to the higher activity and faster deactivation of the first sample.

The AXPD method can be used for investigating zeolites with Si:Al ratios as high as 15 to achieve a quantitative and unambiguous picture of the catalytically active sites. This method can be considered a major advance in the fundamental understanding of the relationship between zeolite structure and its catalytic activity. We believe that AXPD at the Al X-ray absorption edge could become the technique of choice for zeolite scientists interested in pinpointing the active catalytic sites in their materials.

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Talk (12 min)

Pair distribution function analysis – from nanoparticle dispersions to bulk metallic glasses

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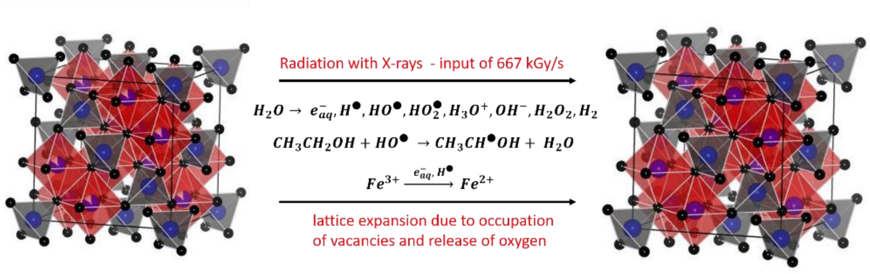
The pair distribution function (PDF), experimentally obtained by Fourier transformation of total scattering patterns, is perfectly suited to study the structural arrangement of materials lacking long-range order.

Previously, high energy X-ray total scattering was applied to investigate aqueous iron oxide nanoparticle (IONP) dispersions, to elucidate the potential presence of hydration shells. By double-difference PDF (dd-PDF) analysis of the total scattering data from the dispersion minus bulk water minus the IONP powder, a strong signal from IONP dispersions freshly re-dispersed after purification was retrieved. This signal suggested the presence of a hydration shell, which is an interfacial region with enhanced ordering of water molecules in comparison to bulk. However, recently this dd-PDF signal has been traced back to ethanol impurities of ca. 6 vol%, which feature local structural motifs in the dilute aqueous dispersions that differ from motifs in bulk ethanol.[1] The developed dd-PDF analysis is therefore a powerful tool to retrieve tiniest signal contributions in multicomponent systems. Further, the little ethanol amount has shown huge impact on beam-induced redox chemistry, visualized below (reprinted from [2]), of the IONPs in the highly brilliant X-ray beam of ESRF-EBS, even at energies of 65 keV.[2]



Already long ago, PDF analysis was used to study e.g. the effect of low-temperature annealing on the nearest-neighbour coordination in metallic glasses.[3] Further, it was shown, that the PDF of small metallic nanoparticles and bulk metallic glasses (BMGs) can be modelled with non-space filling icosahedral clusters with high atom-position disorder.[4] Those PDFs resemble damped sine waves in the intermediate range order, similar to the signal of the dilute ethanol motifs detected in nanoparticle dispersions.[2] Therefore, the gained expertise in PDF analysis will be used, to elucidate potential differences in the local and intermediate range order of BMGs depending on processing parameters, in future.

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Talk (12 min)

Electron Pair Distribution Function - a tool to study local order in poorly crystalline-, nano-, and amorphous materials

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Pair distribution function (PDF) analysis is a key technique for studying highly disordered crystalline, amorphous, and nanomaterials, as it provides information on the short-to-mid range order of materials without assuming any periodic structural model. Although PDF is commonly obtained from X-ray total scattering data at synchrotron facilities, it can also be obtained from electron total scattering data in conventional electron microscopes (TEM) collected from nm^3-sized volumes of the materials to be characterized.[1] Such electron PDF (ePDF) analysis can, in addition, be coupled with further complementary TEM techniques, such as imaging and spectroscopy, enabling the simultaneous acquisition of spatially resolved structural, morphological, and electronic structure information. However, obtaining a quantitative electron total scattering signal presents a significant challenge, as a single elastic scattering approximation of X-ray PDF analysis no longer holds for electrons. Instead, multiple scattering from thick specimens and inelastic scattering from amorphous materials contribute significantly to the electron total scattering signal, thus complicating the subsequent data processing and altering the peak intensities in the obtained ePDF. Moreover, achieving statistical significance in ePDF measurements for a number of crystallites and their crystallographic orientations is hindered by the limited specimen volume probed (≈1 µm size aperture) and the flat configuration of the specimen.

Here, we will first discuss the technical aspects of acquiring reliable ePDF data. Using zero-loss energy-filtered electron diffraction and rotational electron diffraction with precession, we optimized the acquisition of total scattering data for materials with different crystallinity (highly disordered crystalline, nanostructured, amorphous) and geometry of the specimens (with random and preferential orientation of crystallites). Second, we will show how the combined use of ePDFs and TEM imaging allows us to describe the short-range order and structural disorder in two very different materials systems: crystalline metal-substituted polyheptazine imides (PHI) with a high concentration of defects and CeO$_2$ mesocrystals[2]. Moreover, an outlook on the advantages of applying this tandem approach to bimetallic nanoparticles for applications in catalysis will be discussed.

We thank the ETH Zurich, Max Planck Society, and the SNF for financial support.

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Talk (12 min)

Protein crystals as a template for *in situ* formation of magnetite nanoparticles

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Crystallisation in confined spaces is a widespread phenomenon in nature. Many processes like frost heave, biomineralization (bones and seashells), growth of salt and ice crystals in the pores of masonry happen not in a bulk, but in limited volumes. Reducing the volume of the system influences not only the probability of nucleation, but also the kinetic. As the results, in reduced volumes become possible stabilisation of metastable polymorphs, formation of crystals with preferred orientations, modification of morphology, etc.[1]

One of the most fascinating cases of crystallisation in confined spaces – formation of magnetite nanoparticles inside magnetotactic bacteria. The particles have unusual morphologies, homogeneous size and superparamagnetic properties.[2] The control of the magnetite nanoparticles formation could be explained by a combination of physical and chemicals factors in which nucleation and growth of magnetite crystals is performed in confined vesicles (magnetosomes) modulated by the interaction with different proteins.[3]

In this work, we imitate this type of control over the precipitation of magnetite using channels of crosslinked protein crystals (CLPCs). CLPCs with different pore size and amino acid decoration were used to study their influence on the magnetite precipitation. We obtained gradient distribution of nanoparticles with a narrow size distribution of around 2 nm independently of the channel diameter size of the CLPCs. But the pores size influenced the stabilisation of the Fe-rich phase. In case of lysozyme (the smallest pore size), the amorphous metastable intermediates of magnetite were stabilised, while in glucose isomerase crystals, the amorphous phase were recrystallised into the crystalline state of magnetite. Our results demonstrate control in the size and stability of those Fe-rich nanoparticles and the potential use of the CLPCs as excellent scaffolds to study the crystallisation in confinement.

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Talk (12 min)

Host lattice display: a method for the analysis of biomolecules

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Diffraction methods like crystallography and electron microscopy are key technologies in structural biology. As the name implies, crystallography requires crystals to amplify the diffraction of photons, which is not the case for electrons. Unfortunately, growing suitable crystals can be a time-consuming trial and error process without guaranty for success. The host lattice display method (HLD) was developed to support the structural analysis of biomolecules[1]. Here, the molecule of interest is arranged in a regular assembly by means of a host lattice, which is a porous crystal lattice that can be obtained under established conditions. For imbedding the molecule of interest at unique sites in the host lattice we have used designed ankyrin repeat proteins that are fused to a bulky scaffold protein. The method was initially developed to study relatively short peptides, but in principle it is applicable even to large macromolecules[1, 2]. In practice HLD is limited by the temperature factor gradient of the assembly, which is a feature of the host lattice design, and the occupancy of the target molecule.

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Talk (12 min)

Heterogeneous Nucleation on The Eggshell Membrane: Sustainable Development of Biomaterials for Bone Regeneration.

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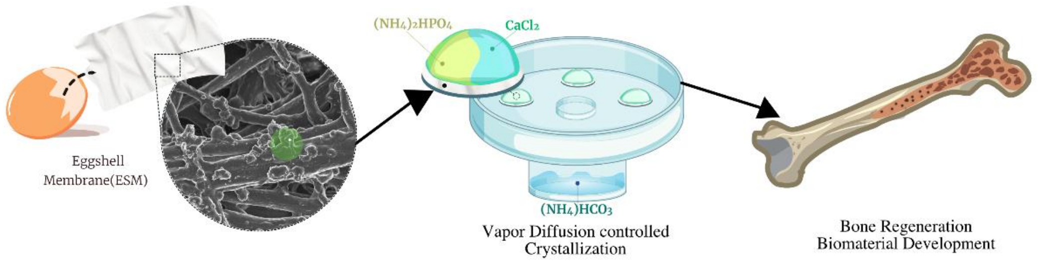
The eggshell membrane serves as a natural template for the heterogeneous nucleation of calcium carbonate in the form of calcite. This results in forming the complex biomineral that makes up the eggshell[1]. Our research team tested the ability of this biopolymeric material to nucleate calcium phosphates, a different type of mineral which this template is naturally designed for. Calcium phosphates constitute the main mineral content of human mineralized tissues, such as bone and teeth[2]. These minerals, mainly apatite, are of particular interest in biomaterial synthesis[3]. With controlled crystallization techniques, such as vapor diffusion crystallization[4], the eggshell membrane can be used successfully as a template to create hybrid materials composed of organic-inorganic interfaces that resemble human mineralized tissues[5]. During the presentation, we will present the results of our experimental observations of the controlled crystallization of calcium phosphate phases on the eggshell membrane, state-of-the-art, and future perspectives for biomaterial development.



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Talk (12 min)

Bridging the gap between Electron and X-ray Diffraction

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Structure determination on ever smaller and more weakly diffracting crystals is one of the biggest challenges in crystallography. Traditionally, in-house X-ray crystallography covers sample sizes down to a lower limit of approximately 50 µm.[1] Consequently, electron diffraction is receiving a lot of attention, as it promises structure determination on significantly smaller samples. However, while micro-ED can cope with samples in the nm range up to approximately 1 µm, the refined structure models are less accurate compared to X-ray data.[2] Furthermore, the preparation of suitable sub-µm samples is often a challenge, whereas few micrometers sized crystals would be readily available. Therefore, equipment for X-ray structure determination closing the gap for samples between 50 to 1 micrometer in size would be highly desirable.

Exciting developments and latest innovations in X-ray source and detector technology enable the crystallographer now to bridge this gap. Crystal sizes in the sub-10 µm range are routinely accessible by modern instrumentation, while at the same time retaining the convenience and accuracy of single crystal X-ray structure determination. This will be highlighted by single crystal X-ray diffraction data collected on three micro crystals and compared to recently published MicroED Data on the same.[3]

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SSCr Annual Meeting 2023: Abstracts for Posters

Poster

Bragg peaks within the Debye scattering equation

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The Debye scattering equation (DSE, (1)) provides the powder diffraction pattern of an ensemble of identical particles, randomly oriented in space with fully uniform distribution, as a function of the coordinates of the atoms within one particle. More precisely, it only depends on the coordinates through the scalar distances between atom pairs. As such, it is an essential tool to calculate the exact diffraction response of a particle, independently if the atomic structure is crystalline or not. For large and perfectly crystalline particles, the diffraction response concentrates on a set of sharp peaks (Bragg peaks) whose position only depends on the 3-D periods of the structure, while the intensity only depends on the structure of the periodically repeated unit (unit cell).

The possibility of encoding Bragg peaks directly into the DSE has not been explored, to my knowledge. It turns out that it is possible. Periodicity along one direction can be described by substituting the sinc terms of the DSE with more complex terms. The expression remains a simple analytical function also for periodic objects with limited lateral extension and a finite number of periods, leading to terms suitable to describe periodicity in finite systems without having to evaluate the 3-D reciprocal space and then project it onto the radial direction.

At this point, this is no more than a curiosity. However, often, when a tool exists, its utility can be later discovered.

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Boris Gruber’s contributions to mathematical crystallography

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Boris Gruber, a Czech mathematician, made fundamental contributions to the study of crystal lattices.

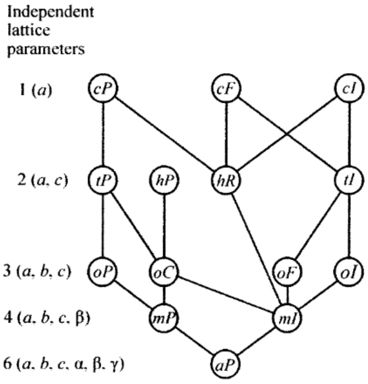
Boris Gruber (1921-2016) at age 90. (Courtesy of his son Jiří Gruber)

There are 14 Bravais types of lattices. The three cubic types (primitive *cP*, face-centred *cF*, body-centred *cI*) have only one free parameter, the edge length *a* of the cubic cell. The hexagonal *hP*, the rhombohedral *hR*, and the two tetragonal types *tP* and *tI* have two free parameters *a* and *c*. The four orthorhombic Types *oP*, *oC*, *oF, oI* have three free parameters *a*, *b* and *c*. The two monoclinic types *mP* and *mI* have four free parameters *a*, *b*, *c* and an angle β. The anorthic type *aP* has six free parameters *a*, *b*, *c* and the angles α, β and γ.

As the number of free parameters is largest for anorthic lattices, it is most important to classify such lattices according to their crystallographic properties. In his paper “Classification of lattices: a new step”[1] Gruber defined 127 “Genera”, which constitute a finer classification than Bravais types. Whereas each of the three cubic Bravais types corresponds to one genus, each of the types *aP* and *mI* split into 43 genera. Lattices of the same genus agree in the densest directions and planes and the symmetry of these planes.

In September 2022 a satellite “MACSMIN 2022” of the 33rd European crystallographic meeting was held in Liverpool, devoted to Crystal Lattice Classifications. Gruber’s results[1] were an early step in this direction.

For all Bravais types except *aP* Gruber determined necessary and sufficient conditions for the free parameters satisfied by the lattices corresponding to a given Bravais type[2]. His results were used by Grimmer to determine the limiting cases of the Bravais types[3].



The Bravais-lattice type of the lattice at the upper end of a line is a limiting case of the type at the lower end.

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Poster

Hirshfeld atom refinement of crystalline systems using periodic kernels

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Hirshfeld atom refinement (HAR) is a method for determining the molecular structures by combining single crystal X-ray diffraction data with *ab initio* calculations of electron density and its partitioning. [1] The partitioning of electron density is described by a weight function defined in direct space. This function represents the ratio of the electron density due to the atom of interest to the sum of electron density contributed by each atom in the system assuming a spherical atomic density. While this methodology has been successful in handling crystals composed of finite molecules, but it has limitations when it comes to dealing with periodic network structures. Here, we propose a framework for partitioning electron density in periodic systems by introducing periodic functional kernels, *e.g.* periodic gaussians which is convolution of gaussian and lattice functions. It has advantages such as rigorously eliminating infinite sums and preserving the local symmetry of Hirshfeld atoms—partitioned aspherical atomic electron density—sitting on high symmetry positions. This approach provides a solid theoretical foundation for conducting HAR in crystalline systems and further deepens our understanding of the behavior of crystal orbitals.

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Poster

Structure – Performance Relationships in Fe_2O_3-based Oxygen Carriers for Chemical Looping Water Splitting

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Chemical looping is an emerging technology to produce high purity hydrogen from fossil fuels or biomass while simultaneously capturing CO_2 on a distributed scale. One of the challenges in this process lies in maintaining the stability and reactivity of oxygen carriers during cyclic processes of reduction and oxidation. Fe_2O_3–Al_2O_3 are candidates for the chemical looping water splitting. However, typically, Fe_2O_3–Al_2O_3 oxygen carriers suffer from decay in H_2 yield with cycle number due to the formation of $FeAl_2O_4$, which has low capacity for water splitting at the operating conditions of conventional chemical looping schemes (700–1000 °C). To address this issue, in this study we investigated the potential of incorporating sodium in the synthesis of Fe_2O_3–Al_2O_3 oxygen carriers to improve their stability during cyclic redox tests. Detailed structural insights into the oxygen carrier were obtained using X-ray powder diffraction (XRD), X-ray absorption spectroscopy (XAS) at the Al, Na, and Fe K-edges, and scanning transmission electron microscopy/energy-dispersive X-ray spectroscopy (STEM/EDX) analyses. The addition of sodium successfully hindered the formation of $FeAl_2O_4$ and instead stabilized the oxygen carrier by promoting the formation of a layered structure known as Na-β-Al_2O_3 phase.[1]

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Understanding green MOF-74 synthesis by high time-resolution XRD and FTIR

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Metal-organic frameworks (MOFs) are promising porous materials for numerous applications in gas separation, gas storage, and catalysis.[1] A notable challenge for the MOF practical implementation is the development of synthetic procedures with speed, scale, and quality matching the industry requirements. Understanding MOF formation pathways is crucial for developing such procedures.

In this work, we studied the mechanism of formation of the MOF-74 family in aqueous solution on a preparative scale (> 0.5 g) using high time resolution (50 ms) powder X-ray diffraction (XRD) and attenuated total reflection IR spectroscopy (ATR-IR). A custom-made stainless steel batch reactor cell equipped with a ZnSe crystal (30°, 50x44x2 mm) and an external loop for XRD data collection was used. Techniques such as Multivariate Curve Resolution (MCR)[2] and time-dependent peak fitting were used to extract information from the data for further processing.

The evolution of FWHM of several characteristic XRD peaks was analyzed via the Williamson-Hall method. Together with the evolution of the lattice parameters, the results indicate that growth of the MOF crystals under the experimental conditions occurs along the *c* axis in the R-3 hexagonal cell. Fitting the XRD intensity data using the Gualtieri model[3] revealed the kinetic parameters of MOF nucleation and growth as well as nucleation probability vs. time, which correlates with the ν(C=C) MOF IR peak width. Coupled with electron microscopy, these observations allowed us to propose a zinc precursor-dependent MOF synthesis mechanism (Figure 1), as well as to establish optimized synthetic protocols for MOF-74 materials.

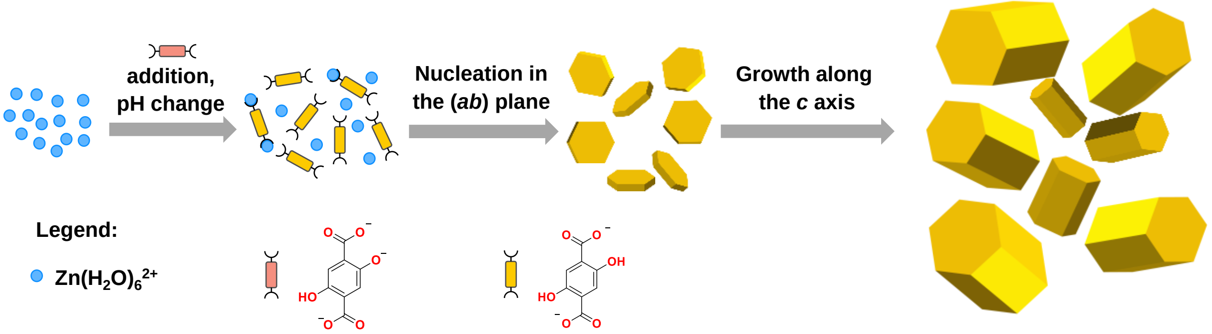

Figure 1. Zn-MOF-74 synthesis mechanism using zinc precursor with non-coordinating anions.

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Poster

Salen-derived multi-metallic complexes

Jocelyn Pradegan and Katharina M. Fromm

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Salen is one of the most studied ligands in chemistry, notably for its straightforward synthesis and its ability to coordinate a variety of metal ions.[1] This Schiff base compound has a N_2O_2 chelate site allowing the coordination of one metal ion. Salen is an interesting ligand in that it can be functionalized providing a panoply of new ligand structures. The main application of salen-metal complexes is in the field of catalysis,[2] the most well-known being the Jacobsen catalyst for its enantioselective epoxidation of alkenes.[3]

In our studies, we aim at synthesizing multi-metallic complexes with two or three different metal ions. To achieve this goal, salen can be functionalized with glycol chains creating e.g. a O_3O_3 recognition site for a second metal ion. The combination of different metal ions can provide enhanced chemical and biological properties.[2] For instance, the synthesized multi-metallic complexes could be used as mixed metal oxide precursors or show potential synergic antibacterial properties.[4]

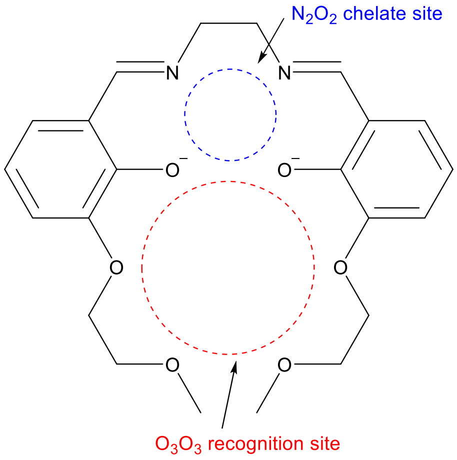

Fig. 1 : Representation of salen-derived ligand with N_2O_2 chelate and O_3O_3 recognition sites

Acknowledgements

The authors acknowledge support from the Swiss National Science Foundation (Project numbers 178827 and 204215).

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(1) Asatkar, A.K.; Tripathi, M.; and Asatkar, D. *IntechOpen* **2020.**
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(3) Hanson, J. *J. Chem. Educ* **2001**, *78*: 1266-1268.
(4) Finelli, A.; Abram, S-L.; Hérault, N.; Crochet, A.; and Fromm, K. M. *Cryst. Growth Des.* **2020**, *20*: 4945-4958.

Minutes of General Assembly 2022: Swiss Society for Crystallography SGK/SSCr

Thursday, 15.09.2022, 13:30 – 14:30
Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Freiestrasse 3, 3012 Bern

Agenda:

1) Determination of the quorum according to Art. 12/by-laws
2) Proposition for acceptance of the minutes of the General Assembly 2021, Fribourg
3) Reports
   a) Annual report
   b) New incentives
   c) Annual financial statement
   d) Budget for next year
4) Elections
   a) Definition of a chairperson for the elections
   b) Confirmation of the present board members (transfer of secretary from Antonio Cervellino to Paula Abdala)
   c) Election/confirmation of the auditors
   d) Confirmation of delegates to Confirmation of delegates to SCNAT, ECA, IUCr, SSC and IOCG
5) 2023 Meeting and General Assembly. Decision on location and organizer (UZH, Bernhard Spingler)
6) PhD Prize 2023 (rules, amount)
7) Other motions of members and communication (please communicate to the president 10 days prior to the meeting)

The minutes of our last General Assembly (University of Fribourg, September 2nd, 2021) are published on page 54-64 (and following) of the SGK/SSCr Newsletter # 108, September 2022.

Minutes:

- Chair: Pascal Schouwink, President
- Chair for the elections: Simon Grabowsky, Vice President
- Keeper of the minutes: Antonio Cervellino, Secretary

Membership 2022:

- 13 Honorary members
- 14 Library members
- 158 Ordinary members (with right to vote)
- 9 Corporate members (with right to vote)

Ordinary members variation with respect to the previous year:

- 146 were already members the previous year.
  2 exits and 12 new ordinary members in 2022.

Corporate members variation with respect to the previous year:

- 8 were already members the previous year.
  1 new corporate member in 2022.

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

The quorum for the validity of the assembly is 10% of the ordinary members (16) and 10% of the corporate members (1). The presence of at least 23 ordinary members was verified (Art. 12). So was the presence of at least two corporate members (DECTRIS Ltd, represented by Dubravka Šišak-Jung; CSEM, represented by Olha Sereda) was verified (Art. 14). Therefore, the quorum was reached, according to the bylaws.

Note: the quorum threshold was prudentially established to be 18 members (10% of ordinary AND honorary members) but this inflated threshold was also amply met.

2) Proposition for acceptance of the minutes of the General Assembly 2021, Fribourg.

VOTING: The minutes of the General Assembly 2021, held in Fribourg, reported in the Newsletter issue # 108, are approved unanimously, without abstentions.

3) Reports

3a) Annual report

The President, Pascal Schouwink, gives an overview of the most important activities of the board of the SGK-SSCr in the past year.

- Website problems at the start of 2022. The old website was hijacked and a ransom was requested; of course this was refused, but it meant that the SGK-SSCr had to build a completely new website https://swiss-crystallography.ch/ With the new website we have also new email contact address swiss.crystallography@gmail.com; and we are happy to announce also the new Twitter account @Swisscrystallog, open of course to all members to announcements of crystallographic interest.
- SGK-SSCr PhD prize: the next edition will be in 2023.
- Flack Crystallographic Lectures: next cycle in November 2022. Announcement in NL # 108.
- Continued support for schools, namely the PSI Powder Diffraction School (last ed. 2021, next edition 2023) and the Zurich Crystallographic School (last edition 2022, next edition 2024).
- Erice Crystallographic School: Dubravka Šišak-Jung has been offered the co-direction.
- Simon Grabowsky organizes SECAM in Lausanne.
- IUCr commissions renewals. The SGK-SSCr nominated the following commission members: Simon Grabowsky, Commission for Quantum Crystallography; Antonia Neels, Commission for Powder Diffraction; Alex Dommann, Commission for Crystallography of Materials; Oksana Zaharko, Commission for Magnetic Structures.
- ECA Board Meeting report (by the SGK-SSCr delegate Tony Linden) :
  - Updated statute to address legal issues in NL, domiciliation country of ECA.
  - Special and General Interest Groups renamed for consistency.
  - New treasurer of ECA is Antonia Neels.
  - Next European Crystallographic School: Berlin 2023, Nancy 2024.
  - Next ECM meetings: ECM 34 Padova (I) 2024, ECM 35 L'viv (UA) 2025. Montenegro is bidding for 2026.
  - Berthaut Young Crystallographers' Prize : too few applications, submissions encouraged.
  - Individual ECA membership encouraged.
- Flack Lectures 2021 (only zoom). Theme: biocrystallography. 7 lectures with different speakers. Quite successful.

- Flack Lectures 2022 in-person. Lukas Palatinus travelling speaker, will take place in November in various Swiss institutions.
- Flack Lectures 2023. Theme/speaker: proposals sought after.

3b) New incentives

- Scholarship for Ukrainian students. Aimed to cover some of the living costs of Ukrainian students. A number of proposals were received, one scholarship assigned this year to Oksana Shlyakhtun. She is due to start a PhD project at EMPA supervised by Davide Bleiner. The scholarship will cover her living costs until the PhD salary will be available.
- Satellite workshop proposal at the IUCr meeting in 2023. The theme will be how to prepare for experiments at synchrotrons. Support from the Commission for Synchrotron Radiation forthcoming. Sponsors (DECTRIS Ltd and others) will be covering part of the costs, a small fee is envisaged for the balance.
- The SGK-SSCr intends to propose organizing the EPDIC conference for 2026. The EPDIC committee is well disposed.
- Report on the SNBL User Meeting in Bern that was well attended (76 participants). Underlined problems with the current funding schemes. The Swiss Chemical Society will be approached in order to join forces and find better solutions together with the Swiss Steering Committee.
- The Annual Meeting 2023 of the SGK-SSCr will take place in September 7 and 8, 2023 in Zurich at the Chemistry Department of the UZH. The first day will be devoted to a 1-day workshop on a theme that will be proposed by students during this meeting.
- The next edition of the PSI Powder Diffraction School will take place In September 2023, from 11-15.9.2023. Then the school’s next edition, that has maintained a biennial cadence since 2008 (last edition in 2020, one year offset due to the Covid pandemic), will not take place before 2026-2027 due to the upcoming shutdown for upgrade of the SLS.

3c) Annual financial statement

Enrico Giannini (Treasurer) presents the closing of the financial year 2021 and the financial situation in 2022.

Summary SGK Finances 2021

	CHF
Total 31.12.2020	**57’795.27**
UBS account	54674.12
Cash on hand	515.55
Total 31.12.2021	**55’189.67**

Balance - 2’605.60

Report of revisors:

The budget 2021 has been approved by the auditors Kurt Schenk and Bernhard Spingler (Geneva, 09.03.2023). Report:

Revisorenbericht für die Jahresrechnung 2021 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. 2021 bis 31. Dez. 2021. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2021 ist der Stand der Konten und der Kasse:

UBS	SFr.	54’674.12
Kasse	SFr.	515.55
Summe SGK	SFr.	**55’189.67**

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

Ort / Datum
Genève, 09.03.2022

Unterschriften

B. Spingler (Universität Zürich)	K. Schenk (EPF Lausanne)
Basel (online)	Signau (on line)
B. Spingler	

SGK Financial Report 2021

Income:

Membership dues:		
Full members (various amounts due to debts)		
2x30 + 1x37.99 + 62x40 + 1x44 + 1x50 + 12x80 + 2x120 + 1x160		4’031.99
Students 9x10 + 1x20		110.00
Companies 6x130 + 1x124 + 1x260		1’164.00
Total membership	5’305.99	
Subsidy SCNaT (2020)		2’247.05
Others (sponsorships…)		500.00
Total Income		**8’053.04**

Expenses:

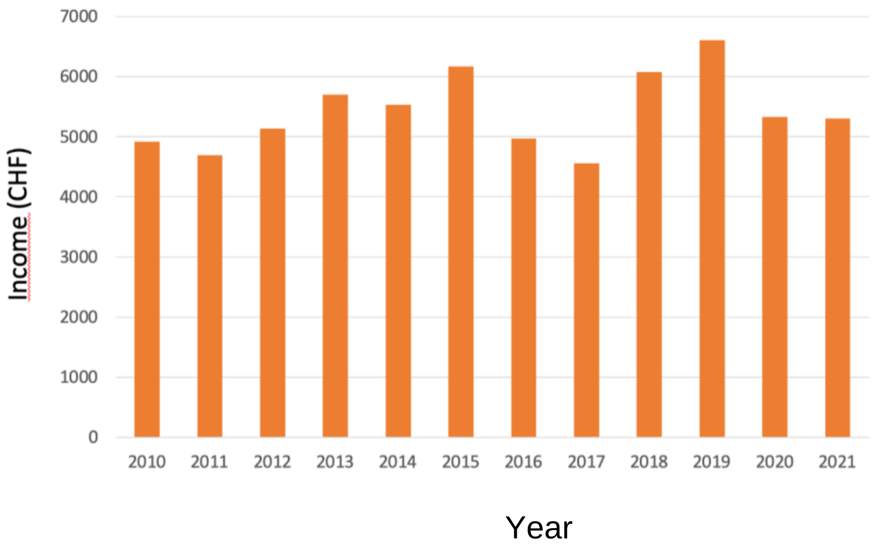
Membership dues to SCNat (166 members at 31.12.2020)		1'162.00
Travel costs of IUCr delegates		1000.00
Annual Meeting		3500.00
Travel Grants (including PhD prize)		**3730.70**
Howard Flack Lecture Series		**0**
Association to ECA	192.94	
Printing and publishing costs (newsletter)		962.10
Website	21.20	
Bank expenses		89.70
Total Expenses		**10‘658.64**
Income – Expenses		**- 2’605.60**

SGK Financial Report 2021

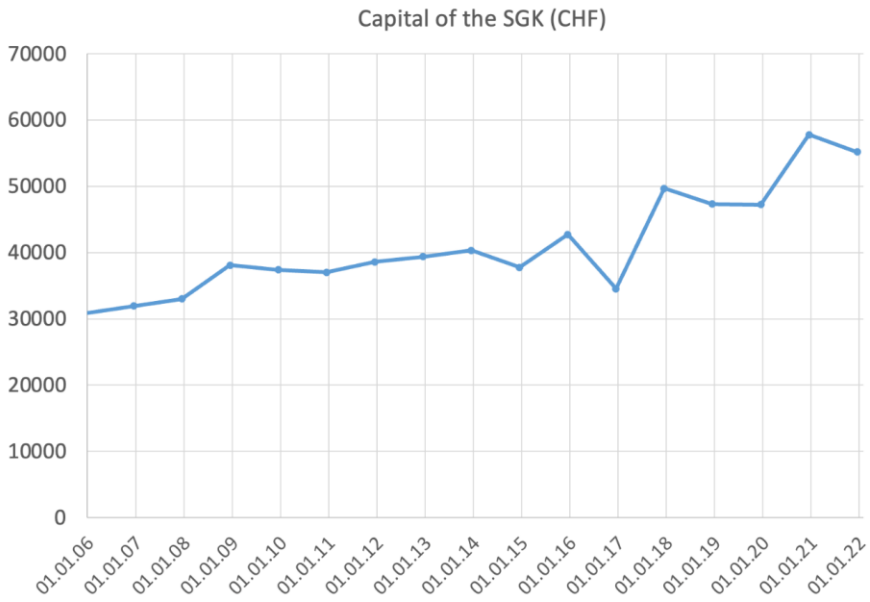
<u>Cash on Hand - 2021</u>:

Status 31.12.2020	**524.40**		
Total Income		0.00	
Total Expenses		8.85	
Balance (Income – Expenses)		0.00	
Starting Balance + Income – Expenses		515.55	
Cash on Hand 31.12.2021			**515.55**

Fluctuations of memberships dues



SGK financial situation 2022

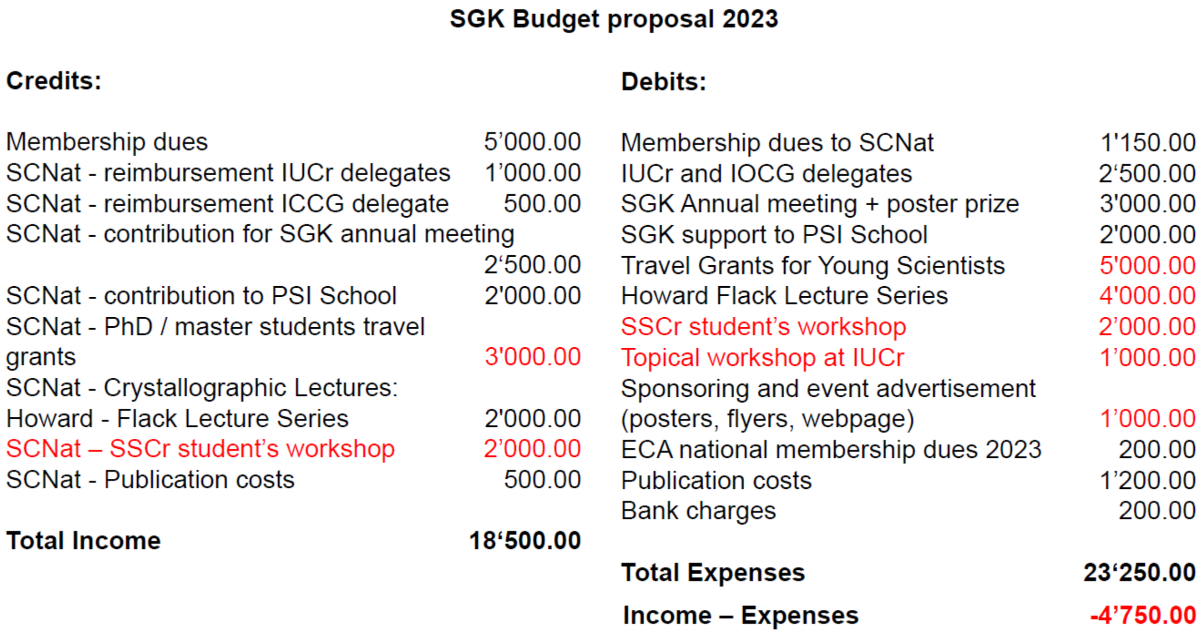


SGK financial situation 2022

Credits:	
Membership dues (until 31/08)	3’988
SCNat contribution 2021 (not yet paid)	6’000
Total Income	**9’988**

Debits:	
SGK Scholarship Ukraine	7’500.00
Zürich School of Crystallography	2’000.00
SGK annual meeting (+ poster prize)	3'000.00
ECA delegate	1’000.00
ENCG delegate	500.00
Travel grants for students	2’000.00
Membership dues to SCNat	1'120.00
Bank charges	33.30
Flack Lecture series (expected)	3’000.00
Publication costs	1’302.00
ECA membership	183.60
Total Expenses	**21‘036.90**

3d) Budget for next year



SGK Budget proposal 2023

Credits:	
Membership dues	5’000.00
SCNat - reimbursement IUCr delegates	1’000.00
SCNat - reimbursement ICCG delegate	500.00
SCNat - contribution for SGK annual meeting	2‘500.00
SCNat - contribution to PSI School	2'000.00
SCNat - PhD / master students travel grants	3'000.00
SCNat - Crystallographic Lectures: Howard - Flack Lecture Series	2'000.00
SCNat – SSCr student’s workshop	2’000.00
SCNat - Publication costs	500.00
Total Income	**18‘500.00**

Debits:	
Membership dues to SCNat	1'150.00
IUCr and IOCG delegates	2‘500.00
SGK Annual meeting + poster prize	3'000.00
SGK support to PSI School	2'000.00
Travel Grants for Young Scientists	5'000.00
Howard Flack Lecture Series	4'000.00
SSCr student’s workshop	2’000.00
Topical workshop at IUCr	1’000.00
Sponsoring and event advertisement (posters, flyers, webpage)	1’000.00
ECA national membership dues 2023	200.00
Publication costs	1’200.00
Bank charges	200.00
Total Expenses	**23‘250.00**
Income – Expenses	**-4’750.00**

Membership fees 2022:
Regular membership fee: CHF 40 / year
Student membership fee: CHF 10 / year
Corporate membership fee: CHF 130 / year.
It is proposed to maintain the same membership fees for the year 2023.

As per the bylaws, the Assembly is required to vote on the presented financial reports and membership fees.
VOTING: The Annual financial report 2022, presented by the Treasurer Enrico Giannini, is approved unanimously, without abstentions.
VOTING: The Budget forecast 2023, presented by the Treasurer Enrico Giannini, is approved unanimously, without abstentions.
VOTING: The prolongation of the current fees for 2023 is approved unanimously, without abstentions.

4) Elections

4a) Definition of a chairperson for the elections

The chair for the elections will be assumed by the Vice President, Simon Grabowsky.

4b) Confirmation of the present board members. Transfer of the Secretary function from Antonio Cervellino to Paula Abdala.

VOTING: The present board members are confirmed unanimously, without abstentions.

VOTING: The transfer of the Secretary function from Antonio Cervellino to Paula Abdala is approved unanimously, without abstentions.

4c) Confirmation of Bernhard Spingler as Auditor. Replacement of Kurt Schenk with Antonia Neels as Auditor.

VOTING: Bernhard Spingler as Auditor confirmed and Antonia Neels as Auditor is replacing Kurt Schenk. The vote is unanimous, without abstentions.

4d) Confirmation of delegates to SCNAT, ECA, IUCr, SSC and IOCG

Delegates proposed:

ScNat:	Pascal Schouwink
ECA:	Tony Linden
IOCG:	Enrico Giannini
IUCr:	Simon Grabowsky, Pascal Schouwink

VOTING: The proposed delegates are approved unanimously, without abstentions.

5) 2023 Meeting and General Assembly. Decision on location and organizer (UZH, Bernhard Spingler)

As already mentioned, the Annual Meeting 2023 of the SGK-SSCr will be organized by Bernhard Spingler (Uni Zurich) in September 7 and 8, 2023 in Zurich. The first day will be devoted to a 1-day workshop for young scientists.

Candidatures for the 2024 meeting are welcome (western Switzerland, Sankt Gallen? Basel?)

6) PhD Prize 2023 (rules, amount)

In 2023 another SGK-SSCr PhD prize will be assigned. Applications are warmly invited. The proze amounts to CHF 2000.- and the deadline is 1.5.2023. The rules will be published on the webpage and the newsletter.

7) Other motions of members and communication

None.

The meeting ends at 14:25, 15.09.2022.

Minutes written by the Secretary, Antonio Cervellino, and approved by the President, Pascal Schouwink.

Investigation of the local structure of nano ZrO_2 and amorphous $Zr(OH)_4$ using PDF analysis

Michael Evans

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The performance of (heterogeneous) catalysts depends strongly on their structure and morphology. Smaller particle size means more surface area and higher activity, but also makes structure analysis with traditional diffraction techniques more challenging. Moreover, many important catalyst materials exhibit polymorphism, and one polymorph may be favored above others for its improved performance.

Zirconium dioxide (ZrO_2) is used in applications involving interactions with CO, H_2, CH_4, CO_2, water, and hydrocarbons [1]. It exists in three crystalline forms: at room temperature the monoclinic $P2_1/c$ phase is most stable, while at higher temperatures the structure transforms to the tetragonal $P4_2/nmc$ (> 1214 °C) and finally cubic Fm-3m (> 2377 °C) phases. The tetragonal phase, which shows improved catalytic properties, can be stabilized at room temperature if synthesized as sufficiently small nanoparticles [2].

Atomic pair distribution function (PDF) analysis has gained popularity in recent years, due to its ability to provide local structure information in disordered, nano, and amorphous materials. Conventional wisdom has been that the technique is too time-consuming and complicated to be done in the home lab. Recent advances in both hardware and software, however, have made PDF analysis faster and more accessible to the average user. Here we present a report demonstrating PDF analysis using a laboratory diffractometer, with measurement times of just a few hours.

Experimental

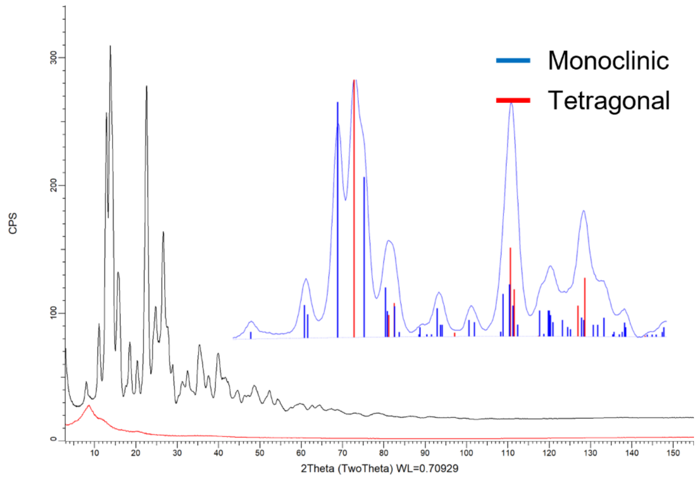

Figure 1: Raw diffraction data of ZrO_2 (black curve) and empty Kapton capillary (red). The insert shows the low angle region, with the blue and red tick marks representing the monoclinic and tetragonal structure of ZrO_2, respectively.

Diffraction data of ZrO_2 powder prepared in a 0.5 mm Kapton capillary and $Zr(OH)_4$ powder prepared in a 1.0 mm Kapton capillary were collected on a D8 ADVANCE equipped with a Mo sealed tube source, focusing Goebel mirror optic, capillary stage, and an EIGER2 R 500K detector placed at a distance of 118mm from the sample to maximize scattered intensity. A 2θ scan from 3 to 155° 2θ (Q = 0.47 to 17.3 $Å^{-1}$) was done with the detector in 1D mode. An empty Kapton capillary was measured and removed as background, and the total measurement time was 2 hours for ZrO_2 and 4 hours for $Zr(OH)_4$. Generation of the PDF from raw data and PDF refinement were done using the software package DIFFRAC.TOPAS V7 [3].

Results

The ZrO_2 sample contains both the monoclinic and tetragonal polymorphs, which can be seen in the raw diffraction patterns (Figure 1). Because of the broad diffraction peaks due to small crystallite size, an accurate Rietveld refinement can be challenging on such a sample. PDF analysis, however, can provide a more detailed picture, especially about local structure, crystallite domain size, and phase fractions.

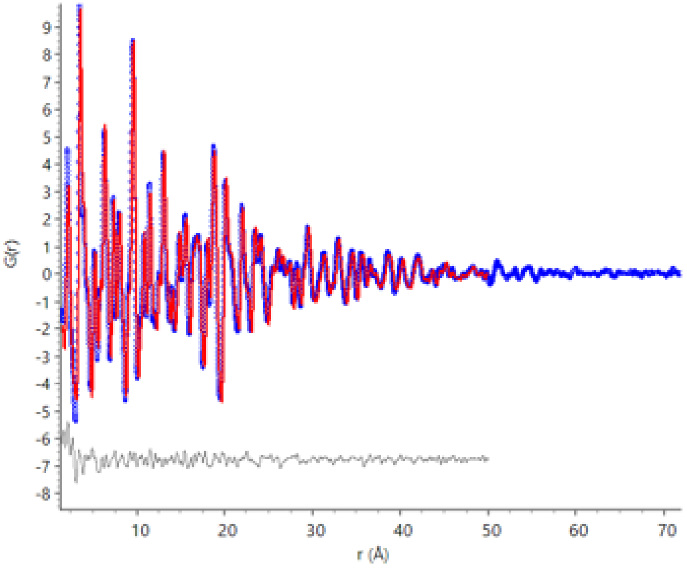

Figure 2: PDF refinement on ZrO_2 with 2-phase model.

Figure 2 shows the PDF refinement on ZrO_2 (blue curve) using a 2-phase model containing both monoclinic and tetragonal ZrO_2. The final quantitative analysis result shows that the sample contains 62.5% monoclinic ZrO_2 and 37.5% tetragonal ZrO_2, with domain sizes of 6.6 and 6.3 nm, respectively. Qualitatively, the signal in the experimental PDF has gone to 0 by around 65 Å, meaning there are no more atom-atom correlations beyond this distance, which agrees with the refined domain sizes.

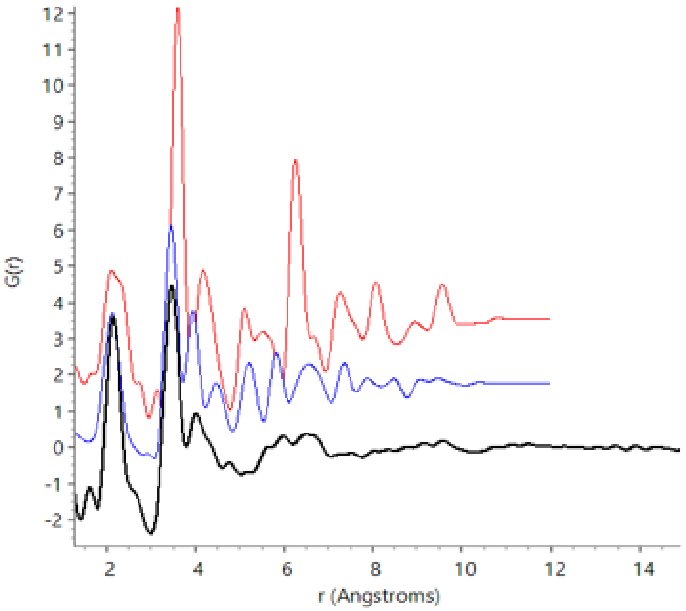

Figure 3: Experimental PDF of amorphous $Zr(OH)_4$ (black curve), and the calculated PDFs of monoclinic ZrO_2 (blue) and tetragonal ZrO_2 (red).

One can also take a more qualitative approach to evaluating the PDF data. Figure 3 shows the experimental PDF of $Zr(OH)_4$ (black curve), along with calculated PDFs of monoclinic ZrO_2 (blue curve) and tetragonal ZrO_2 (red curve) assuming a 10 Å domain size. Beyond 10 Å the structural coherency disappears, and the PDF curve goes to zero, which is typical for amorphous samples. Comparing the calculated PDFs against the experimental one, it appears that the local structure of $Zr(OH)_4$ agrees more closely with monoclinic ZrO_2, especially below 4 Å. This implies that the local coordination of Zr and O atoms in amorphous $Zr(OH)_4$ is quite similar to that of m-ZrO_2 (7-coordinated Zr-O), and that the domains are very small (less than 1 nm).

Conclusion

Pair distribution function analysis is an ideal technique for investigating the local structure of amorphous and nanocrystalline materials, and the experiments can be carried out in just a few hours on modern laboratory X-ray diffractometers.

Acknowledgements

Samples courtesy of Dr. Matthew Suchomel, ICMCB-CNRS, Pessac, France.

References

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PDF measurement: from large-scale facilities to the laboratory

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**Correspondence: gwilherm.nenert@malvernpanalytical.com*

Introduction

The atomic Pair Distribution Function (PDF) contains information about the structural correlations present in a material. For crystalline materials with no disorder, the Rietveld method has been tremendously useful in probing the structure of materials. With the rise of nanostructured and/or disordered materials, the Rietveld method fails to describe the structure at the local level and prevents a full characterization of the materials properties. Many of those materials even appear as what is called X-ray amorphous: they exhibit large halos with no sharp features. The PDF method offers the great advantage to give access to structural information irrespective of the nature of the material. This method has been around for long time within the liquid and glass community but is rather recent in the nano-materials community. Many publications are presenting and explaining the advantage of this method and we refer the general reader to the already existing literature for some general description/introduction to the method1,2. In this contribution, we aim to discuss the various points to take into consideration when carrying PDF measurements on a laboratory system.

From the large-scale facilities to the laboratory

The necessity to measure large Q range for PDF analysis requires hard radiations. For long time, this has been available only at large scale facilities. However, with the development of hard radiation laboratory X-ray sources (Ag or Mo radiations for instance) and suitable high-power generators (60 kV), PDF analysis became available on laboratory instruments. The first report on PDF measurements using a standard laboratory diffractometer was back in 2009 using a scintillation detector[3]. Some of the key parameters to obtain meaningful data were already mentioned: a proper shielding of the optical path to achieve feature-free background and variable counting time strategy to improve signal/background ratio at high Q. Following up this initial work, it has been shown that a variety of materials could be investigated in the lab depending on their level of absorption ranging from soft condensed matter (such as C_{60} fullerene) or hard materials such as CeO_2 requiring Ag radiation (E~ 22 keV)[4]. Comparison of PDF measurements between laboratory and synchrotron radiation have shown that data of comparable quality could be obtained[5].

Experimental set-up and data evaluation

The necessity to measure large Q range for PDF analysis requires hard radiation and thus best suited X-ray tubes would be Mo (λ = 0.71 Å, Q_{max} ~ 17 Å^{-1}) or Ag (λ = 0.56 Å, Q_{max} ~ 22 Å^{-1}). The choice between those 2 tube anodes is governed by the required resolution of the experiment ($\delta = \pi/Q_{max}$, 0.18 vs 0.14) and the absorption of the sample. Additionally, one may consider the cross-section difference between Mo and Ag radiation. Due to those considerations, Mo radiation would tend to be preferred for low absorbing samples while Ag radiation would tend to be preferred for heavy absorbing samples. To make the most sensible data reduction to generate the F(Q), the chemical composition of the sample and the instrument geometry need to be considered and are fully supported within the HighScore suite[6]. An example of the typical experimental set-up is shown in Figure 1 and the corresponding F(Q) achievable data quality is shown in Figure 2. As the generation of ripples (termination ripples, noisy data, etc) is inherent to the Fourier transformation of the F(Q) to obtain the G(r), it is of prime importance to minimize the noise level at high Q as it contains important structural information. Consequently, the most adequate and relevant evaluation of the collected data quality of the F(Q) is the signal/noise ratio at Q_{max}. As illustrating in Fig. 2, the achievable noise level can be very low.

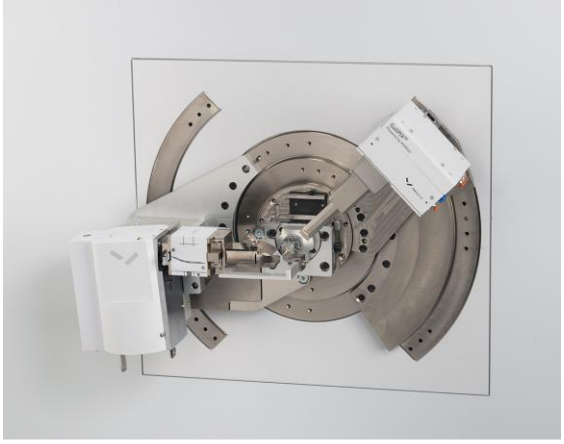

Figure 2. Typical experimental set-up for PDF measurement: hard radiation tube (Mo or Ag), a focusing mirror, capillary spinner, antiscattering device combined with a highly efficient detector (CdTe, GaliPIX^{3D})

After having collected high quality F(Q) data, the data are corrected as specified previously to give rise to the G(r). We present in Figure 3 the resulting G(r) obtained from the F(Q) presented in Figure 2 and its corresponding fit to the tetragonal SnO_2 structure. Data correction and the PDF fitting were done using the HighScore suite[6].

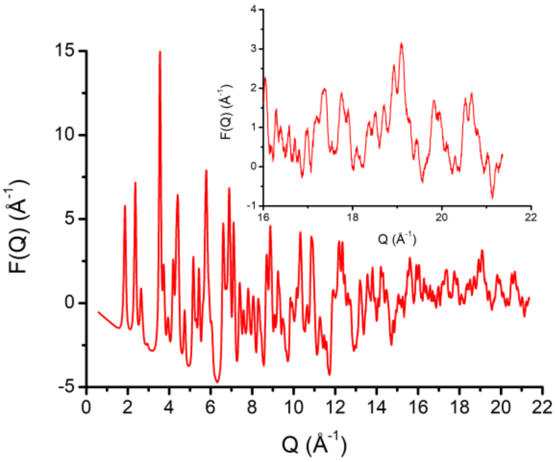

Figure 2. High quality experimental F(Q) as illustrated by low noise level at high Q collected on nano-SnO_2.

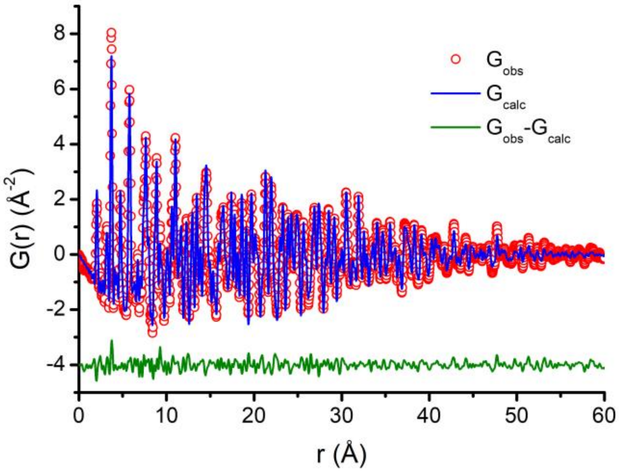

Figure 3. Corresponding G(r) of the F(Q) shown in Fig. 2 and corresponding PDF fitting (R_{wp} = 14%).

Conclusions

The technical development of hard radiation tubes, high power generator, high efficiency detector (CdTe technology for instance) combined to proper shielding made possible to carry out PDF measurements in the laboratory. The noise level of the F(Q) at high Q values is decisive for the data quality of the PDF measurement.

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Report on the Summer School on Diffraction and Crystallography, BM01-ESRF

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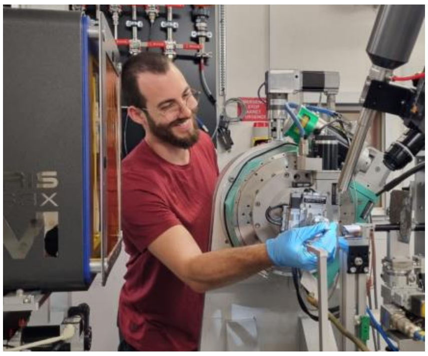
The first Swiss SNBL at ESRF BM01 Summer School on Diffraction and Crystallography was held in Grenoble, 05-09 June 2023. The school was proposed by Swiss members of the Swiss-Norwegian Council Wendy Lee Queen (EPFL) and Paula Abdala (ETHZ), who also organized financial support and educational certification. Sixteen students from ETHZ and EPFL attended the school to explore the theoretical and practical aspects of advanced structural characterization of crystals, powders and thin films. The school included lectures, tutorials and practical exercises demonstrating the benefits of synchrotron diffraction data for various facets of materials science. At lectures organized by BM01 staff, students got familiar with the basics of synchrotron science, diffraction and crystallography. Particular attention was paid to the information content of diffraction data, data processing, in-situ and operando experiments. The students also presented their research projects, the presentations were followed by a discussion on the possible diffraction experiments that could help answering the underlaying scientific questions. As a part of practical exercises, the students measured their own samples including in-situ structural evolution of powder materials during a chemical reaction, textured films of MOFs and solar cell compounds, and single crystals with correlated disorder. The students were hence exposed to a wide variety of projects, the final lesson was allocated for a discussion on how to write and submit proposals for synchrotron experiments.



The portfolio of experimental techniques available at BM01 currently includes a set of synchrotron diffraction tools such as small-angle scattering, wide-angle scattering, high resolution diffraction, reciprocal and direct space diffraction mappings. We hope that the School helps Swiss material scientists to benefit from these synchrotron tools in their research. More information can be found at www.snbl.eu. Proposal deadlines are 1st of March and 10th of September.

Dr. Diana Piankova, postdoctoral researcher at ETH Zurich

Department of Mechanical and Process Engineering

“The synchrotron school at ESRF in Grenoble, organized by enthusiastic scientists from BM01, provided a rare opportunity to learn about synchrotron techniques through informative lectures and hands-on experience in sample measurements. Not only were we able to perform high-resolution powder diffraction, GIXRD, and single crystal

measurements on our samples, but we also had the chance to conduct in situ experiments under a gas environment with the necessary high temporal resolution to probe the kinetics of different processes.

As an electron microscopist, I found this school particularly valuable. It allowed me to expand my expertise beyond electron radiation-based methods and provided insights into implementing synchrotron techniques in my research, enabling a multiscale understanding of functional materials. By the end of the school, we had gained knowledge of the capabilities of the BM01 beamline for studying our materials, laying a strong foundation for future proposal planning and identifying the research questions that can be effectively addressed using synchrotron radiation. We are extremely grateful for this experience, made possible by the exceptional team of Dmitry, Chloe, and Charlie, who shared their knowledge and provided their support and help throughout the school.”

PhD student Ghewa Alsabeh,

EPFL Laboratory of Photonics and Interfaces and Smart Energy Materials, Adolphe Merkle Institute, University of Fribourg

“The synchrotron summer school was a one of a kind experience for me! It was the first time I ever saw and worked with such a big and powerful synchrotron. Seeing how these measurements take place in real life was amazing and prepared me well for my next beamtime application and measurements!

Such a high-brilliance photon beam allowed me to learn more information about the perovskites I am studying due to the high accuracy of light diffraction from it. I was able to prove the formation of 2D phase, study the phase purity, the orientation of the materials and get much more information.

Besides this, I had the chance to engage with a team of experts in the field to discuss my project and the obstacles I am facing for a better understanding of my material. Huge thanks go to BM01 staff for their assistance not only during the school but also in the after-school follow-ups!”

SGK/SSCr Travel Grants 2023: January - July

We congratulate Maximilian Krödel and Rohan Pokratath for their travel grants in 2023. Hereby, the awardees share their impressions of the scientific meeting in which they participated.

ACS Spring Meeting 2023 by Maximilian Krödel (ETH Zürich)

26-30th March 2023, Indianapolis, USA

Chemistry is at a crossroads. Sustainable approaches for chemical synthesis and processes have to be developed to make us ready for the future. This was the topic of the ACS Spring Meeting 2023 in Indianapolis (USA), which I recently had the opportunity to present my work at as part of my PhD program at ETH Zürich. The conference gathered a broad spectrum of researchers in the chemical sciences, focusing on topics ranging from crystallization of viruses in liquid aerosol droplets to green synthesis of organic molecules.

As part of a session focused on the atomic-scale understanding of CO_2 capture, I presented our work on the promotion and deactivation mechanisms of Na_2CO_3-promoted CaO-based sorbents for CO_2 capture. As this research has been a long time in the making (> 3.5 years), it was a great experience to present it to a panel of distinguished scientists in the field, and receive insights into novel aspects of CO2 capture. Specifically, learning about the application of ionic liquids as well as high surface area porous salts (Erich Bloch) for CO_2 capture led to fruitful discussions, setting our lab up to use these materials in the future.

The conference was packed with up to 50 talks in parallel, including talks by startups and companies on how they plan to transform new scientific findings into commercial products. This allowed me to learn about fields that were completely new to me, e.g. the deactivation of viruses in aerosol droplets or the characterization of radical species in fuels. As far the commercialization of technologies goes, I really enjoyed the concept of Carbon Limit to use enhanced weathering of an alkaline earth metal oxide-based additive in cements for long-term storage of atmospheric CO_2. Beyond this, there were plenty of opportunities to network with fellow researchers in a friendly atmosphere.

Maximilian Krödel during his presentation

I am very grateful for the support of the SSCr / SGK with a travel grant that allowed me to attend this conference. It really helped me broaden my view on the future of chemistry as well as the role of crystallography and made me even more motivated to continue with my own research to contribute to it.

UK Colloids 2023 by Rohan Pokratath

17 - 19 July 2023, Liverpool, United Kingdom

The UK Colloids 2023 conference was a remarkable event that brought together leading scientists, researchers, and industry professionals from around the world to discuss the latest advancements in the field of colloids. The conference spanned over three days, featuring insightful plenary presentations, themed sessions, and thought-provoking poster sessions. As a speaker, I had the privilege of participating in this enriching experience, broadening my knowledge, and engaging with fellow enthusiasts. My presentation was scheduled in the afternoon with the nanoparticles and nanostructured materials themed session, and I was eager to share my work with fellow researchers in the field. After my talk, I had the opportunity to network with fellow researchers who shared similar interests. Many attendees approached me to discuss my research in more detail, offering constructive feedback and suggestions for future studies. These interactions were invaluable as they provided new perspectives and opened the door to potential collaborations.

Rohan Pokratath

One of the highlights of the conference was the poster session, where researchers showcased their recent work. The poster session provided an excellent opportunity for researchers from different backgrounds and specialties to engage in fruitful discussions. The industry exhibitions at the conference were bustling with activity, featuring booths from various companies dedicated to colloidal science and its applications. Each exhibitor presented their latest products, technologies, and services, tailored to meet the needs of researchers and industries utilizing colloidal systems. Engaging in discussions with representatives from different companies enabled me to learn about the latest advancements in the field, potential collaborations, and upcoming trends. The interactions were not only informative but also highlighted the significance of bridging the gap between academia and industry.

Attending the UK Colloids 2023 conference was a memorable and valuable experience. The conference provided a platform to learn about cutting-edge research, connect with experts in the field, and gain a broader perspective on colloidal science. The interactive sessions, talks, and networking opportunities have left a lasting impact on my professional development. I am grateful for the opportunity to be part of this esteemed event and look forward to applying the knowledge gained to contribute meaningfully to the field of colloids in the future.

Ukrainian Students' Scholarship

In solidarity with Ukrainian students leaving in Switzerland the SSCr announce in May 2022 an extra-ordinary scholarship aiming at covering some of the living costs of these students. One scholarship was assigned to Oksana Shlyakhtun. Her application was supported by Prof. Davide Bleiner (Empa). Here she tells us about her scientific projects.

A contribution to the Newsletter by Oksana Shliakhtun

Since the 9th f March, I am a Ukrainian refugee in Switzerland. The war caught me being a Ukrainian researcher working at the Lebedev Research Institute, in Moscow. Immediately, I left Russia, seeking a safe haven to complete my study and continue a scientific career.

I was enrolled as a visiting Master's student at the University of Zurich (UZH) and working at Empa (Swiss Federal Laboratories for Materials Science and Technology) at the same time. Here, I worked on the design and calculation of the wide-range XUV spectrometer for plasma applications, joining the project of Dr. Di Qu - at that time Ph.D. student in the laboratory for Advanced Analytical Technologies. My work focused on the design of a flat-field spectrometer optimized for wavelength range and the desired size of the spectrometer itself, calculating focal planes and spectral resolution. I presented the results at the 6th Meeting of the Swiss Analytical Scientist and at the Colloquium Spectroscopicum International XLII.

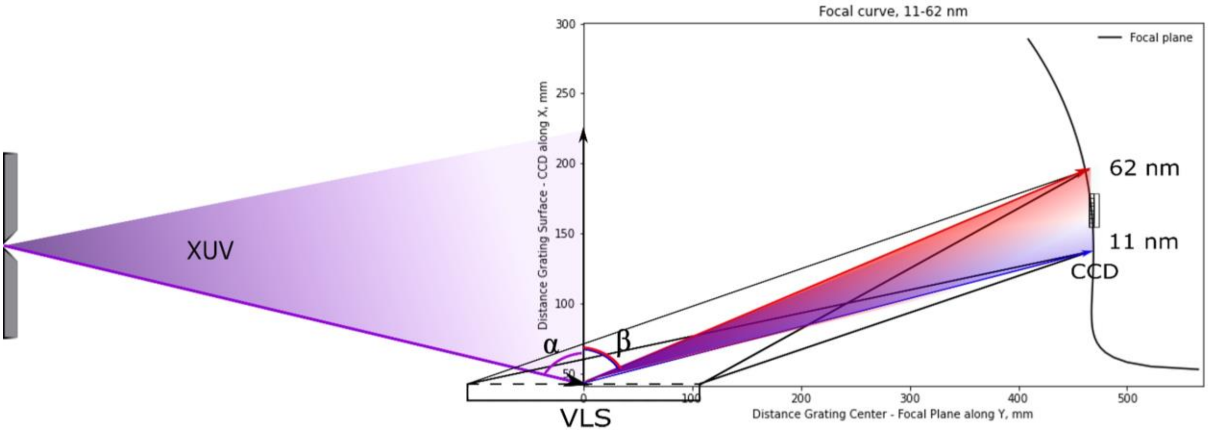


Fig. 1 Schematic drawing of a flat-field XUV spectrometer with a calculated focal curve

Starting in September 2022, I am officially enrolled as a Master's student at UZH. In November, I started my Master's project in the Correlated Quantum Matter Group at Paul Scherrer Institute (PSI) and I joined the Sample Environment Group for an apprenticeship at PSI. My future thesis will be related to neutron scattering experiments on a new quantum simulator.

This year in Switzerland, I had the opportunity to continue my scientific career and gain experience in cutting-edge research laboratories. I would like to thank my colleagues at Empa and PSI for the invaluable support that I received from them.

I am grateful to the Swiss Society for Crystallography for granting me the opportunity to give my small contribution to world science!

Lecture Series 2023

Swiss Society for Crystallography
Howard Flack Crystallographic Lecture Series

Local Order and Pair Distribution Function Analysis

Prof. Simon Billinge
Columbia University, New York

Biography

Prof. Billinge has more than 25 years of experience developing and applying techniques to study local structure in materials using x-ray, neutron and electron diffraction including the development of novel data analysis methods including graph theoretic, artificial intelligence and machine learning approaches. He earned his Ph.D in Materials Science and Engineering from University of Pennsylvania in 1992. After 13 years as a faculty member at Michigan State University, in 2008 he took up his current position as Professor of Materials Science and Applied Physics and Applied Mathematics at Columbia University and held a joint position of Physicist at Brookhaven National Laboratory between 2008 and 2022.

Prof. Billinge has published more than 350 papers in scholarly journals. He is a fellow of the American Physical Society and the Neutron Scattering Society of America, a former Fulbright and Sloan fellow and has earned a number of awards including the 2022 Distinguished Powder Diffractionist Prize of the European Powder Diffraction Conference, the 2018 Warren Award of the American Crystallographic Association and being honored in 2011 for contributions to the nation as an immigrant by the Carnegie Corporation of New York. He is Section Editor of Acta Crystallographica Section A: Advances and Foundations. He regularly chairs and participates in reviews of major facilities and federally funded programs.

Abstract

Nanoparticles, nanoporous materials and nanostructured bulk materials are at the heart of next generation technological solutions in sustainable energy, effective new pharmaceuticals, and environmental remediation. Their study involves going beyond traditional crystallography to understand local arrangements of atoms on different length-scales. These lectures will explore this problem, and describe recent developments in solutions based on total scattering methods such as the atomic pair distribution function (PDF) method. They will explore the state of the art in time and spatially resolved studies of heterogeneous samples, operando measurements from operating devices, developments in ultra-fast pump-probe PDF measurements using x-ray free electron lasers, and latest approaches in data interpretation using machine learning and artificial intelligence.

The approaches will be illustrated with examples from a wide range of materials science problems from batteries and catalysts, to quantum materials with emergent behaviours, to next generation pharmaceuticals. We will also explore the philosophical question of whether materials have a genome, and if they do, what might we use it for.

Swiss Society for Crystallography

Howard Flack Crystallographic Lecture Series

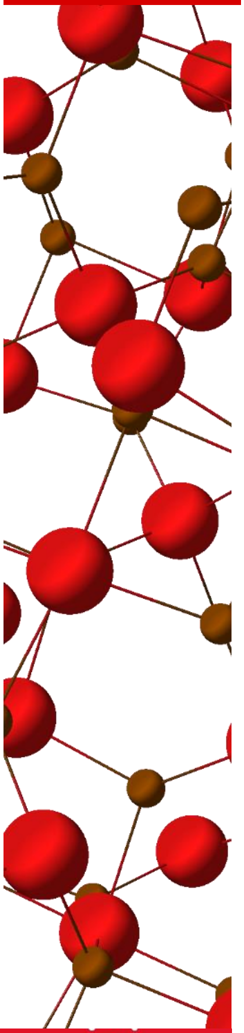
Local Order and Pair Distribution Function Analysis

Prof. Simon Billinge
Columbia University, New York

Schedule November 6 - 10

📅	📍
Monday **6**	**EPFL, Sion**
Tuesday **7**	**University of Bern, Bern**
Wednesday **8**	**University of Basel, Basel**
Thursday **9**	**ETH Zürich, Zurich**
Friday **10**	**Dectris AG ., Baden** **Paul Scherrer Institute, Villigen**

SSCr PhD prize



The Swiss Society for Crystallography PhD prize 2023 will be announced in the SSCr Annual meeting.

The SSCr board thanks the PhD panel of expert reviewers for evaluating the 2023 PhD Award.

Travel Grants for SGK/SSCr Scientists

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

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

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

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

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

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

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

Financial support can also be granted to retired SSCr members:

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

Meetings, Conferences, Workshops, Schools, Courses

SSCr-SGK Annual Meeting and Workshop

📅 7 - 8 Sep 2023
📍 Zurich, Switzerland,
💻 www.swiss-crystallography.ch

Summer School “Advanced methods for the characterization of applied materials”

📅 25 - 27 Sep 2024
📍 Mülheim an der Ruhr, Germany
💻 https://event.mpi-muelheim.mpg.de/summerschool2023/

SAS2024: The XIX edition of the International Small-Angle Scattering Conference

📅 3 - 8 Nov 2024
📍 Taipei Taiwan
💻 https://www.nsrrc.org.tw/ViewNews/DigestLayout01.aspx?ViewID=D20230517111454305&Lang=Chinese

📅 17 – 29 Jun 2024
📍 Zurich, Switzerland,
💻 www.chem.uzh.ch/linden/zsc/

Calls for proposals at large scale facilities

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

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

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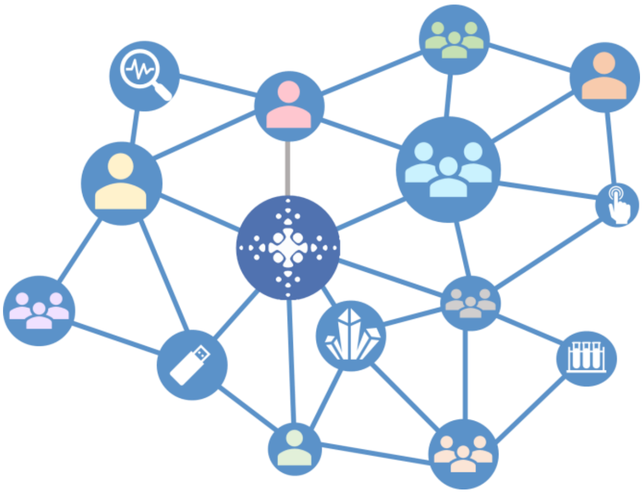

- ✓ Connect with researchers, scientists, and students from across scientific fields.
- ✓ Take part in events organized by the society.
- ✓ Drive the future activities of the society.
- ✓ Benefit from travel grants and PhD awards.
- ✓ Benefit from a network providing access to new collaborations and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

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

Connect with us!

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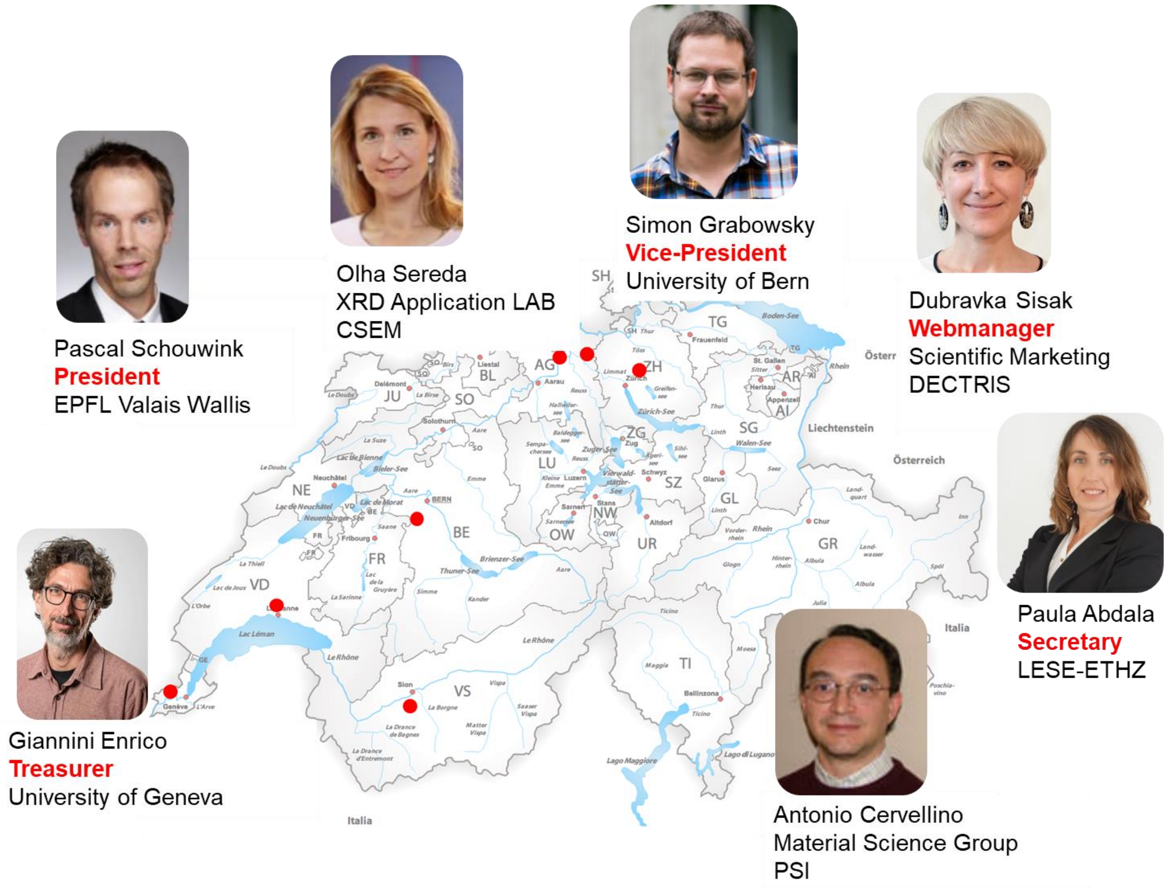

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SGK / SSCr Newsletter No. 110 (2023)