



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

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



## SGK / SSCr NEWSLETTER

ISSN 1662-5358 (printed edition)

ISSN 1662-534X (electronic edition)

**No. 114**  
August 2025



Swiss Society for Crystallography  
Annual Meeting 2025

“Materials Discovery”



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## The President's Page



Dear members,

Beside many exciting scientific contributions, this year's Annual Meeting offers two highlights: the award of the PhD Prize to Yevheniia Kholina and the award of two honorary memberships to Hans Grimmer and Hans-Beat Bürgi. I want to congratulate all three awardees. Yevheniia Kholina has presented an outstanding thesis with the title "Correlated disorder in Prussian Blue analogues: from understanding to control of the local structure" to the jury. This year, the jury had an especially difficult job as they had to read through six excellent theses who were all in the final round, and all six of them would have been worthy PhD Prize winners. I sincerely thank the jury consisting of Radovan Černý, Lynne McCusker, and Florian Kleemiß who

have put a lot of effort and time into the selection process for the sake of our Society.

Hans Grimmer and Hans-Beat Bürgi have been members of the Society for more than 50 years. They have shaped the Society in various functions over the years (President, Secretary, Editor of the newsletter, Organizer of the Annual Meeting, etc.) and with their active participation in nearly every Annual Meeting since the early 1970s. Their scientific contributions and contributions to discussions have always been an enriching part of the Society's life; an Annual Meeting without them is hardly thinkable. Both of them have voiced that the social aspect of the Annual Meeting and the Society as such have been very important to them. I have been a member since 2019 only, a ridiculous six years in comparison, but the rich and very welcoming Society life, including all the social events, has become very dear and important to me, too. Since 2019, we have manoeuvred the Society through the Corona crisis and the Ukraine war, which meant for us to use Society savings to help Ukrainian master students to settle in Switzerland. I believe that as a Society we have such a societal responsibility, and it is very important that we continue to live tolerance and inclusiveness in times where slander of minorities and individuals have become accepted again.

One of such events that combines science with social aspects are the Howard Flack Lectures. This year, Robert M. Hazen from Carnegie Science, Washington D.C., will visit us and give lectures on Mineral Evolution and Mineral Informatics. He is one of the top mineralogists in the world, but he will touch on many aspects of general crystallography, physics, or computer science as well. I am sure that his lectures will be highly exciting for a broad audience. He will speak at Zurich, PSI, Bern, Lausanne, and Geneva between November 10th and 14th. A more detailed schedule can be found in this edition of the newsletter, and later with times and locations of lecture halls on our website [swiss-crystallography.ch](http://swiss-crystallography.ch).

I am looking forward to seeing many of you in Lausanne in September and at the Flack lectures in November.

Simon Grabowsky



## Annual Meeting Swiss Society for Crystallography Scientific Programme

10 September 2025

<b>08:30</b>		Registration and Welcome Coffee
09:20	Welcome address	Arnaud Magrez and Pascal Schouwink
09:30 – 10:30	<b>Materials at Extreme Conditions</b>	Chair: Henrik Ronnow
09:30 – 10:00	High-Pressure Crystallography as a Tool for Materials Discovery	Invited speaker: Natalia Dubrovinskaia (University of Bayreuth, Germany)
10:00 – 10:15	Uniaxial Control of Cuprate Superconductors	Gediminas Simutis
10:15 – 10:30	Understanding and tuning the electronic structure of covalent organic frameworks	Michelle Ernst
10:30 – 11:00		<b>Coffee break, posters, exhibition</b>
11:00 – 11:10	<b>SSCr PhD Prize Ceremony</b>	<b>PhD Award</b>
11:10 – 11:45	Correlated disorder in Prussian Blue analogues: from understanding to the control of the local structure	Award Lecture: Yevheniia Kholina
12:00 – 14:00	<b>General Assembly in room SG0211</b>	<b>Lunch, posters, exhibition</b>
13:00 – 14:00		<b>General Assembly of the SGK-SSCr</b>
14:00 – 14:30	<b>Award of honorary memberships</b>	Hans-Beat Bürgi, Hans Grimmer
14:30 – 15:30	<b>Bulk materials discovery and crystal growth</b>	Chair: Arnaud Magrez
14:30 – 15:00	Crystal Chemistry and Exotic Properties in some Low-D 6th block Transition Metal Phosphates (Cr, Mo, W)	Invited speaker: Olivier Mentré (University of Lille, France)
15:00 – 15:15	Stabilizing Metastable I-V <sub>2</sub> O <sub>5</sub> via Pillaring: Single-Crystal to Single-Crystal transformations for Advanced Lithium-Ion Cathodes	Sarbejeet Chakraborty
15:15 – 15:30	Discovering Vitrification Pathways in Zr-Based Metallic Glasses: Structural Insights from Microgravity Experiments	Damien Terebenec
15:30 – 16:00		<b>Coffee break, posters, exhibition</b>
16:00 – 17:00	<b>Nanomaterials and Disorder</b>	Chair: Raffaella Buonsanti
16:00 – 16:30	Probing Structural Defects and Dynamic Disorder in Halide Perovskite Nanocrystals	Invited speaker: Federica Bertolotti (University of Insubria, Italy)
16:30 – 16:45	SAXS-guided Design of Responsive Microemulsion	Elisa Mégroz
16:45 – 17:00	Disorder structure determination by 3D $\Delta$ PDF analysis of a Dy-based metal-organic framework	Stefano Canossa
17:00		Poster prize, farewell, lab tours

Our sponsors



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**Abstracts of the SGK / SSCr Annual Meeting 2025**

Invited talks

## High-Pressure Crystallography as a Tool for Materials Discovery

Natalia Dubrovinskaia, Leonid Dubrovinsky

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Materials behavior in confined environments often differs significantly from what scientists observe when exploring chemical reactions or phase transformations at atmospheric pressure. In this talk, we delve into high-pressure and high-temperature crystallography as a powerful tool to unravel the effects of extreme conditions on solid matter *in situ*.

We have experimentally investigated various compound classes, including oxides, borides, carbides, nitrides, halides, and hydrides. These studies offer new insights into how extreme pressure-temperature conditions reshape our understanding of matter, revealing novel principles that govern material behavior. A key highlight of this research is the synthesis of compounds with homoatomic anions, representing a groundbreaking advancement in materials design.

The talk will cover both the methodological and technical aspects of high-pressure crystallography, including innovative devices and software for XRD data processing. The implications of high-pressure crystallography extend beyond a single discipline, influencing fields such as physics, chemistry, materials science, earth sciences, and planetary sciences. We will present a critical analysis of how extreme pressures and temperatures challenge conventional chemical norms, highlighting the profound impact of our approach on multidisciplinary scientific research.

## Crystal Chemistry and Exotic Properties in some Low-D 6<sup>th</sup> block Transition Metal Phosphates (Cr, Mo,W).

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This presentation focuses on 6<sup>th</sup> group transition metal phosphates (W, Mo, Cr), characterized by a range of oxidation states from +II to +VI. We will explore the new series of layered monophosphate tungsten bronzes (L-MPTB)  $[\text{Ba}(\text{PO}_4)_2]\text{W}_m\text{O}_{3m-3}$  ( $2 \leq m \leq 5$ ), consisting of m-layer-thick slabs of  $\text{WO}_6$  separated by large spacers. They all show metallic behaviour down to 1.8 K without clear evidence of instability, despite the vicinity of 1D nested topology [1]. Their genuine 2D-character is even more reinforced by the participation of mainly a central W-layers, assigned to anti-polar displacements [2]. Their oxidation under air lead to a series of W and Mo polymorphs that we have using evolutionary crystallographic algorithms (USPEX) and ab-initio DFT calculations. A special attention will be also given to chromium(II) compounds, where the rare  $\text{Cr}^{2+}$  oxidation state is stabilized by the inductive effect of phosphate groups. This, coupled with the Jahn-Teller effect, gives rise to a variety of frustrated crystal structures and spin-lattice interactions. Besides the non-collinear magnetic structures of  $\alpha$ - and  $\beta$ - $\text{Cr}_3(\text{PO}_4)_2$  the incorporation of large cations (e.g. Ba) induces several low-dimensional structures with various exotic features. For instance, the 2D  $-\text{Sr}_2\text{Cr}(\text{PO}_4)_2$  compounds exhibits a two-step layer-by-layer magnetic ordering with significant spin-lattice couplings, finally breaking the structural time-reversal symmetry of the room-temperature crystal structure [3].

Reference to a journal publication:

[1] H. Nimoh *et al.*, *Angew. Chemie Int. Ed.* 2023, 62, e202302049.

[2] H. Nimoh *et al.*, *JACS* 2024, 146, 23955.

[3] H. Nimoh *et al.*, *Inorg. Chem.* 2024, 63, 44, 21000.

## Probing Structural Defects and Dynamic Disorder in Halide Perovskite Nanocrystals

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Lead halide perovskites (LHP) are long-known crystalline materials with  $ABX_3$  general formula (where  $A=Cs^+$ ,  $MA=CH_3NH_3^+$  or  $FA=CH(NH_2)_2^+$ ,  $B=Pb^{2+}$  and  $X=Cl, Br, I$ ), characterized by a three-dimensional  $[PbX_6]^{4-}$  framework and a large A cation residing in the cuboctahedra cavities. These materials in the form of nanocrystals (NCs) are considered ideal candidates to be integrated into television displays and LEDs [1]. Due to the dynamic nature of the perovskite lattice, preventing the charge carriers from trapping, LHP NCs are highly tolerant to structural defects and surface states, which are considered benign with respect to their electronic and optical properties [2].

The flexible nature of the perovskite framework, very prone to structural defectiveness, coupled with the reduced size of crystalline domains, makes these materials unsuitable for conventional crystallographic methods. For this purpose, total scattering techniques based on the Debye Scattering Equation (DSE), have been established as effective methods for characterizing nanoscale materials and taking into account size-induced structural defects, emerging upon downsizing [3]. Through the DSE-based method developed by some of us [4], starting from real-space atomistic models, structural and microstructural information on NCs can be simultaneously derived within a unified approach, with all the well-known advantages associated with the use of reciprocal space methods.

In this talk, experimental and modeling aspects related to the DSE approach applied to provide atomic-to-nanometer scale insights on key nanoscale features of LHPs will be presented, both in steady-state conditions and involving forefront ultrafast pump-probe experiments [5].

A broad spectrum of structural and morphological features of LHPs, unveiled through a synergic combination of reciprocal space methods based on the DSE, will be analyzed, from their peculiar structural flexibility [6], defectiveness [7], to faceting and surface termination [8], to the formation of self-organized superstructures [9,10].

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[2] Kovalenko M. V., Protesescu L. and Bodnarchuk M.I., Science (2017), 358, 745.

[3] Bertolotti F., Dirin D.N., Ibáñez M., Krumeich F., Cervellino A., Frison R., Voznyy O., Sargent E.H., Kovalenko M.V., Guagliardi A. and Masciocchi N., Nat. Mater. (2016), 15, 987 and references therein.

[4] Cervellino A., Frison R., Bertolotti F. and Guagliardi A., J. Appl. Cryst. (2015), 48, 2026.

[5] Yazdani N. et al. Nat. Phys. (2024), 20, 47-53

[6] Bertolotti F., Dengo N., Cervellino A., Bodnarchuk M. I., Bernasconi C., Cherniukh I., Berezovska Y., Boehme S. C., Kovalenko M. V., Masciocchi N., Guagliardi A., Small Structures (2024), 5, 2300264.

[7] Bertolotti F., Protesescu L., Kovalenko M. V., Yakunin S., Cervellino A., Billinge S.J.L., Terban M.W., Pedersen J.S., Masciocchi N. and Guagliardi A., ACS nano (2017), 11, 3819.

[8] Bertolotti F.; Nedelcu G.; Vivani A.; Cervellino A.; Masciocchi N.; Guagliardi A.; Kovalenko M.V. ACS Nano 2019, 13, 12, 14294-14307

[9] Bertolotti F.; Vivani A.; Ferri F.; Anzini P.; Cervellino, A.; Bodnarchuk M.I.; Nedelcu G.; Bernasconi C.; Kovalenko M.V.; Masciocchi N.; Guagliardi A.; ACS nano (2019), 13, 14294-14307.

[10] Boehme S. C. et al. ACS nano (2023), 17, 2089-2100.

*Acknowledgment: Partial financial support by the project "Novel SUSTainable double PERovskites: multiscale characterization from the atomic structure to functional properties (SU-PER)" funded by the MUR Progetti di Ricerca di Rilevante Interesse Nazionale (PRIN) Bando 2022.*

## PhD Award

**Correlated disorder in Prussian Blue analogues: from understanding to control of the local structure**

Yevheniia Kholina, Arkadiy Simonov

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While disorder is often perceived as random and unwanted, in crystals, it is usually correlated on a local scale and can even enhance material properties. In this work, we demonstrate that such correlated disorder in solution-grown Prussian Blue analogue crystals (PBAs) can be systematically manipulated through crystallization parameters that affect growth kinetics—temperature, precursor concentration, chelating agents, and gel media. This control allows us to achieve defect correlation lengths ranging from short-range to long-range, which directly impacts optical anisotropy, gas sorption capacity, and framework stability without altering chemical composition.

We also discovered that not only is crystallization kinetics important but also the crystal growth direction. [1] Defects tend to align anisotropically along growth directions, creating macroscopic domains with lower symmetry than the symmetry one can extract from an average structure based on Bragg peaks. By growing crystals along different directions, we can modify the symmetry and thus properties like birefringence.

Disorder can also be responsive: local structure can undergo transformations triggered by post-synthetic treatments without detectably changing the average structure. We demonstrate that these modifications in PBAs can be achieved by treatments like dehydration or freezing. Dehydration induces an irreversible reshuffling of the vacancy network from a checkerboard arrangement to diagonal channels, altering transport pathways and improving pore connectivity. Similarly, when rapidly cooled, these crystals develop a reversible corrugated structure as water freezes within their pores. These "hidden" phase transitions, invisible to conventional Bragg diffraction, significantly impact material properties, including dehydration kinetics, symmetry, and optical anisotropy.

Our findings transform correlated disorder from an uncontrolled variable into a design parameter complementing standard compositional tuning approaches. The principles developed here extend beyond PBAs towards other solution-grown crystalline systems, particularly metal-organic frameworks (MOFs) and related porous materials, opening new possibilities for engineering materials with tailored properties by controlling their local structure.

[1] Kholina, Y.; Weber, T.; Bang, J.; Baroni, A.; Liebi, M.; Gorfman, S.; Biran, I.; Warren, M.; Chernyshov, D.; Simonov, A., arXiv preprint arXiv:2502.05936. **2025**

## Award of honorary memberships

### **Memories of my relations with the Swiss Society for Crystallography**

Hans Grimmer

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Foundation of the Swiss Society for Crystallography (SSCr) in 1969.

How my interests changed from mathematical physics to crystallography.

Start and early development of the SGK/SSCr Newsletter.

The European Crystallographic Meeting ECM30 in Basel.

Finally, I shall show how much I owe to Howard Flack.

## 60 Years in chemical crystallography (1965-2025)

Hans-Beat Bürgi

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The presentation will focus on a few things that impressed me during those 60 years and a few topics where I think I contributed to the development of chemical crystallography. To put things into perspective the different topics are related to the time line of solutions of the phase problem. A glimpse will be given of the means available for single crystal structure determination during my thesis work (1965-1969) and - more importantly - of the problems that required structural information.

By the 1970s enough information was available to study the correlated deformations of a given structural fragment embedded in different environments (structure correlation). Such studies - based initially on literature searches in the library - were reported from the 1970s to the 1990s in most crystallographic meetings. With the help of structural databases and their associated software (CSD, available online in CH since 1977, and ICSD, PDB) such studies may now be done in a days or so. The best known example of such correlations is a detailed description and discussion of the approach of a nucleophile to an electrophilic carbonyl C-atom[1,2]. The only aspect left in 2025 of this study is the so-called 'Bürgi-Dunitz angle'.

Another topic is atomic displacement parameters  $U_{ij}$  (ADPs, more accurately intra-atomic ADPs,  $U(n)_{ij}$ ). determined for every structure nowadays and representing  $\sim 2/3$  of the information characterizing a crystal structure. ADP information is hardly ever interpreted to any significant degree. This is partly due to a complete lack of information on the correlations of atomic motions (inter-atomic ADPs  $U(mn)_{ij}$ ). Due to the quantum chemical nature of atomic motion and due to anharmonicity of such motion, information on inter-atomic ADPs can be retrieved from multi-temperature data[3]. I consider this result my most original finding. It has, however, had a very modest echo in the crystallographic community.

Work on disorder, diffuse scattering and evolutionary algorithms started when Thomas Weber joined the lab as a postdoc[4]. After retirement (>2007) I continued these studies in collaboration with Tony Linden at UZH and Omar Yaghi at UC Berkeley and I would pursue them further if I had another crystallographic life. Mark Spackman and Dylan Jayatilaka (both from UWA) introduced me to quantum crystallography and let me collaborate in the development of the quantum-chemistry based Hirshfeld Atom Refinement (HAR)[5]. Another topic i am very interested in but never had an opportunity to delve into is crystal nucleation and growth.

Overall, working for 60 years in chemical crystallography with gifted students and brilliant colleagues was a great and satisfying experience.

[1] Bürgi H.B., Dunitz, J.D., Shefter, E., *J. Amer. Chem. Soc.* (1973) **95**, 5065-5067

[2] Bürgi, H.B., Lehn, J.M., Wipff, G., *J. Amer. Chem. Soc.* (1974) **96**, 1956-195

[3] Bürgi, H.B., Capelli, S.C., *Acta Cryst.*, (2000) **A56**, 403-412

[4] Weber, Th., Bürgi, H.B., *Acta Cryst.*, (2002) **A58**, 526-540

[5] Capelli, S.C., Bürgi, H.B., Dittrich, B., Grabowsky, S., Jayatilaka, D., *IUCrJ* (2014) **1**, 361-379

## Contributed talks

## Uniaxial Control of Cuprate Superconductors

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Quantum matter is characterised by competing and intertwined orders. Here I will present our recent advances in using uniaxial pressure as a clean “surgical” tool to tune quantum phases while simultaneously obtaining microscopic insights via scattering experiments. The realizations of the experiments are achieved through technical developments by minimizing the background and enabling the tuning in-situ [1]. First, we study spin order in cuprate superconductors characterized by small moments, which remains challenging for pressure studies. We overcome this challenge by designing a low-background uniaxial strain cell, optimizing the experiment based on neutron-tracing simulations and using aggressive focusing and energy analysis. We show that the spin order parameter in cuprates is uniaxial and coupled to the charge channel [2]. We further show how superconducting transition temperature is affected by uniaxial pressure applied in different directions by combining uniaxial pressure and polarized neutron scattering [3]. To achieve the fine-tuning in-situ, we have designed a new in-situ uniaxial device for largescale facility research based on an actuator-motor mechanism, efficient feedback loops and the sample-holder design enabling rapid exchange of the samples [4]. I will demonstrate the advanced capabilities of this device by reporting the control of charge and structural degrees of freedom as studied by X-rays in an archetypical cuprate [5,6].

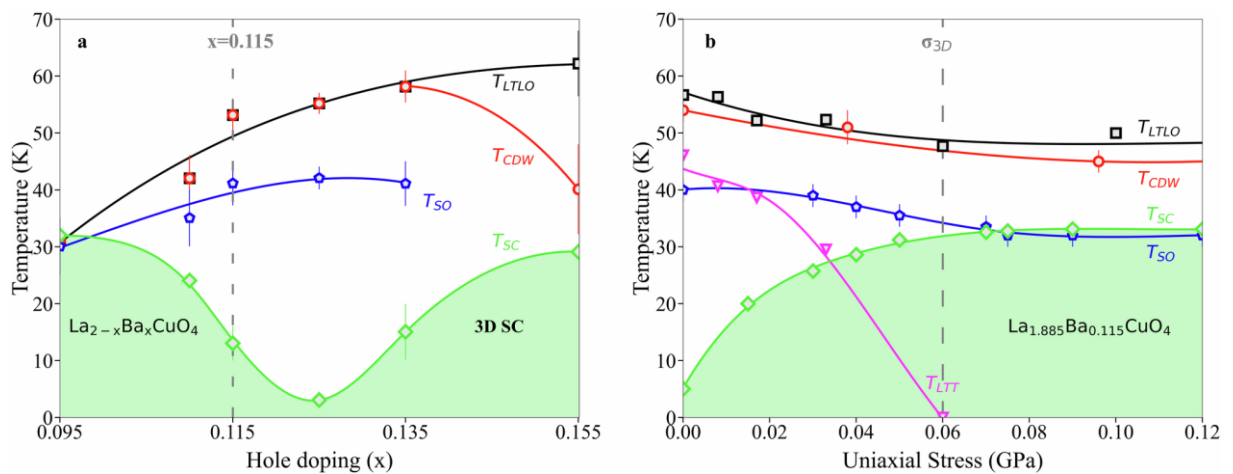


Figure 1- Phase diagram of a La-based cuprate, showing the multiple electronic and structural phases and indicating with a gray dashed line the part of the slice of a phase diagram that was explored using uniaxial tuning. The green area represents phase space where three-dimensional superconductivity (3D SC) is established and the solid lines are guides to the eye of the onset temperatures of charge density wave (TCDW), spin order (TSO) and low-temperature less-orthorhombic (TLTLO) crystal structure. b The complete phase diagram as a function of uniaxial stress, around the doping of  $x = 0.115$ , where the multiple degrees of freedom and corresponding phases are modified. As superconducting temperature is increased with stress, the transition temperatures of charge density wave and spin order are suppressed, together with the reduction of macroscopically occupied volume fraction. Notably, the structural low-temperature tetragonal (LTT) phase is completely suppressed at moderate stress, yet the electronic stripe order persists throughout the studied pressure range, albeit with a reduced volume fraction. All changes saturate above the meager stress of  $\sigma_{3D} \approx 0.06$  GPa [6].

- [1] Simutis et al., Swiss Neutron News 62, 14 (2023)
- [2] Simutis et al., Communications Physics 5, 296 (2022)
- [3] Küspert et al., Communications Physics 7, 225 (2024)
- [4] Simutis et al., Review of Scientific Instruments 94, 013906 (2023)
- [5] Guguchia et al., PNAS 121 (1) e2303423120 (2023)
- [6] Thomarat et al., Communications Physics 7, 271 (2024)

## Understanding and tuning the electronic structure of covalent organic frameworks

M. Ernst (1), R. Fedorov (2), A. Calzolari (3), G. Gryn'ova (4), J. Hutter (5), S. Battaglia (5)

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Covalent organic frameworks (COFs) are crystalline, porous materials composed of light elements connected by strong covalent bonds. Their extended  $\pi$ -conjugation and tunable topologies make them promising for electronic and optoelectronic applications. However, understanding and predicting their electronic structure remains challenging due to the interplay between local building block chemistry and extended topology. This challenge is reinforced by the limited number of experimentally realized COFs and the difficulty of synthesizing well-ordered single crystals, which complicates structural characterization.

I will present two recent studies, in which we applied computational methods to rationalize and tune the electronic properties of COFs.

The first part will focus on how far the electronic structure of a COF can be understood from its molecular building blocks. While fragment-based approaches are well established for metal-organic frameworks, they are harder to apply to COFs, where covalent bonds form a continuous network and electron delocalization is not easily confined to individual subunits. We developed **deCOFpose**, an **automated fragmentation algorithm that identifies chemically meaningful units using a set of graph-based rules**. Applied to over 300 experimentally reported COFs, this approach enables large-scale analysis of the **relationship between fragment frontier orbital energies and full-framework band gaps**. The analysis shows that fragment electronic properties alone do not capture the electronic structure of the periodic COF. Improved correlations emerge when the dataset is restricted to chemically similar subsets, highlighting the combined influence of local chemistry and extended topology.[1]

The second part will address how **hydrostatic pressure and metal intercalation change the band structure** of COF-1, a prototypical two-dimensional framework. Compression up to 10 GPa results in a continuous band gap reduction of approximately 1 eV, which is larger than typically observed in other two-dimensional materials. Metal intercalation induces even more pronounced effects, and, in some cases, a transition to metallic behaviour. These findings demonstrate that pressure and intercalation are effective strategies for tuning the electronic structure while preserving the overall framework connectivity.[2]

Together, these studies illustrate different routes toward a deeper understanding and more systematic control of electronic properties in COFs, relevant to their application in electronic, sensing, and energy-related technologies.

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[2] Ernst, M., Hutter, J., Battaglia, S. (2025). Preprint: ChemRxiv (doi: 10.26434/chemrxiv-2025-4vprm)

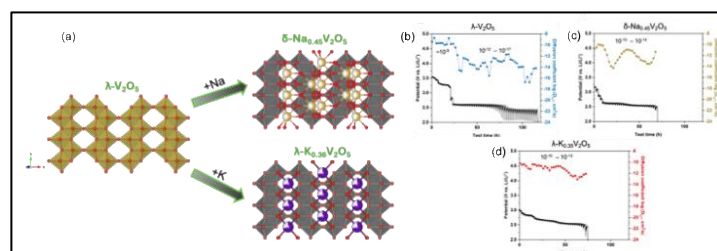
## Stabilizing Metastable I-V<sub>2</sub>O<sub>5</sub> via Pillaring: Single–Crystal to Single–Crystal transformations for Advanced Lithium–Ion Cathodes

Sarbajeet Chakraborty<sup>1,2\*</sup>, Yu-Hsiang Chiang<sup>1,2</sup>, Sarbajit Banerjee<sup>1,2</sup>

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The growing demand for high-performance lithium-ion batteries necessitates cathode materials with enhanced stability and energy density. Vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) has emerged as an enticing candidate, offering high theoretical capacities (~441 mAh/g), but the structural degradation experienced by the thermodynamically stable polymorph,  $\alpha$ -V<sub>2</sub>O<sub>5</sub>, during cycling precludes it from application. Instead, we are exploring the metastable polymorphs of V<sub>2</sub>O<sub>5</sub> and utilizing pre-intercalation strategies to improve the host's structural resilience, using single-crystal electrochemistry to probe ion diffusion at the atomic scale. This approach is particularly effective in layered frameworks, where the strategic insertion of cations expands the host's interlayer spacing as means towards mitigating ion diffusion bottlenecks and suppressing shear transformations. We are currently investigating single crystals of a metastable, double-layered I-V<sub>2</sub>O<sub>5</sub> polymorph synthesized via topochemical routes. Its wide (~8.5 Å) interlayer spacing enables the pre-intercalation of Na<sup>+</sup> and K<sup>+</sup>, producing a pillared structure with enhanced structural rigidity. The single crystals were subsequently topochemically treated to insert Li<sup>+</sup> ions and subsequently *ex situ* single-crystal X-ray diffraction provided the exact crystallographic positions of the Na<sup>+</sup> and K<sup>+</sup> ions, as well as the topochemically inserted Li<sup>+</sup> cations. Notably, the I-K<sub>x</sub>V<sub>2</sub>O<sub>5</sub> phase exhibits significantly reduced lattice distortions compared to the empty I-V<sub>2</sub>O<sub>5</sub>, underscoring the stabilizing effect of the inserted pillaring ions. This enhanced stability is also reflected in the electrochemical studies, which show that I-K<sub>x</sub>V<sub>2</sub>O<sub>5</sub> achieves superior capacity retention and cyclability. Galvanostatic Intermittent Titration Technique (GITT) measurements reveal Li<sup>+</sup> diffusion coefficients several orders of magnitude higher than those in conventional I-V<sub>2</sub>O<sub>5</sub> phases. Ergo, single-crystal-to-single-crystal topochemical transformations reveal ion-specific responses. For example, Li<sup>+</sup> intercalation induces Na<sup>+</sup> rearrangement but does not affect the K<sup>+</sup> ions, demonstrating the nuanced role of the pre-intercalated ions in governing transport kinetics and rate performance. By leveraging structural insights at the atomic scale, our work elucidates ion coordination environments and lattice dynamics in layered oxides. These findings lay the foundation for the rational design of next-generation cathodes with improved performance metrics.



**Figure 2.** (a) Topochemical insertion of double-layered V<sub>2</sub>O<sub>5</sub>. The depicted crystal structures were obtained from single crystal diffraction of the herein synthesized for the empty  $\lambda$ -V<sub>2</sub>O<sub>5</sub>,  $\delta$ -Na<sub>0.45</sub>V<sub>2</sub>O<sub>5</sub>, and  $\lambda$ -K<sub>0.36</sub>V<sub>2</sub>O<sub>5</sub>, viewed down the *b*-axis. (Color key: Na, yellow; K, purple; polyhedral, VO<sub>5</sub>). Li-ion diffusivity of (b)  $\lambda$ -V<sub>2</sub>O<sub>5</sub>, (c)  $\delta$ -Na<sub>0.45</sub>V<sub>2</sub>O<sub>5</sub>, and (d)  $\lambda$ -K<sub>0.36</sub>V<sub>2</sub>O<sub>5</sub> measured by GITT. Black empty circles represent potential variation as a function of discharge/charge. Solid marker with solid line represents Li-ion diffusivity.

## Discovering Vitrification Pathways in Zr-Based Metallic Glasses: Structural Insights from Microgravity Experiments

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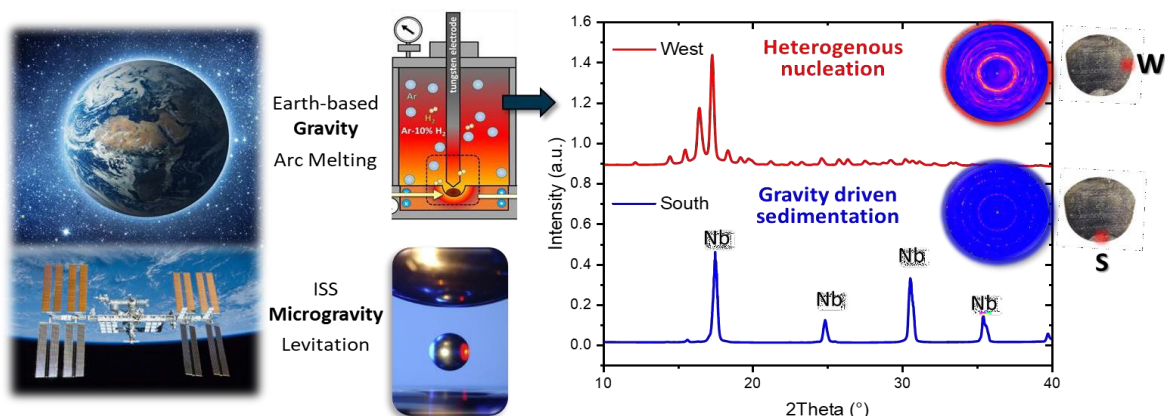
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Bulk metallic glasses (BMGs) offer a compelling route in materials discovery, enabling the design of new non-crystalline metallic alloys with exceptional strength, elasticity, and corrosion resistance.**[1]** These properties stem from their disordered atomic structure, which deviates from traditional crystalline metals and opens new frontiers for applications in extreme environments such as aerospace, energy, and defense.

This study investigates the structural evolution and glass-forming behavior of the Zr-based alloy Vit106a ( $Zr_{58.5}Cu_{15.6}Ni_{12.8}Al_{10.3}Nb_{2.8}$ ) under varying processing conditions. Emphasis is placed on containerless electromagnetic levitation (EML) experiments conducted aboard the International Space Station (ISS), where microgravity enables the elimination of heterogeneous nucleation and gravity-driven segregation. Complementary thermophysical measurements, including viscosity, surface tension, and specific heat, were combined with structural analysis via X-ray diffraction (XRD) and wide-angle X-ray scattering (WAXS) on samples processed both terrestrially and in space.

Key findings reveal that Earth-based processing introduces Nb segregation and premature crystallization, hindering vitrification (see **Figure 1**). In contrast, containerless microgravity conditions facilitate deeper undercooling and reduced nucleation, enhancing amorphous phase formation. Remarkably, thermal modulation in the supercooled liquid state led to an 85 K drop in crystallization onset, suggesting a reversible liquid structural transition that alters nucleation kinetics. Viscosity measurements further confirmed a strong-to-fragile transition in the liquid, underscoring significant rearrangements in atomic mobility. These insights demonstrate the importance of liquid-state control in advancing the discovery and fabrication of new metallic glass materials.



**Figure 1-** Comparison of Zr-based bulk metallic glass (BMG) Vit106a processed on Earth via arc melting and under microgravity using electromagnetic levitation aboard the ISS. The WAXS patterns obtained in transmission mode for the Earth-processed sample reveal signs of heterogeneous nucleation at the edges (red curve) and Nb-rich phase segregation due to gravity-driven effects (blue curve), both of which hinder the formation of a fully homogeneous amorphous structure.

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## SAXS-guided Design of Responsive Microemulsion

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Microemulsions are mixtures of water, oil, surfactant, and co-surfactant that spontaneously self-assemble into nanostructures depending on composition and environmental conditions.<sup>1</sup> They are thermodynamically stable and, depending on the curvature of the surfactant/co-surfactant layer can exist as oil-in-water coexisting with excess oil, water-in-oil with excess water, or bicontinuous systems with oil and water dissolved in a single phase. While the phase behavior of these systems have been studied for decades, typically varying composition, temperature or ionic strength, the formation of food-grade, stimuli-responsive microemulsions that can switch reversibly between these states remains a challenge.<sup>2</sup>

In this presentation, we demonstrate the formulation and characterization of novel, pH-responsive microemulsions using food-grade, polar lipids.<sup>3</sup> The interfacial tension between oil and water in these microemulsions is studied with spinning drop tensiometry, and their nanostructures in solution and as thin films coated onto surfaces are analyzed using Small-Angle X-ray Scattering (SAXS) and Grazing-Incidence SAXS (GISAXS) combined with numerical data modelling. These techniques enable a detailed understanding of how self-assembly and interfacial behavior are influenced by compositional and pH changes. Finally, we examine how these findings contribute to understanding phase transitions in complex fluids and how such systems hold potential for applications in nutrient extraction.

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## Disorder structure determination by 3D $\Delta$ PDF analysis of a Dy-based metal–organic framework

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A novel lanthanide MOF, UoB-100, containing Dy based metal nodes was found disordered in its average crystal structure. Inspection of the diffraction planes reconstructed from laboratory single crystal X-ray diffraction data revealed structured broad intensities containing information on the local arrangement of cluster disorder. A combination of single crystal 3D delta pair distribution function [1] and Monte Carlo simulations afforded a realistic nonperiodic model for the atomic structure of UoB-100, which reproduces the total scattering observed in diffraction experiments [2]. This case study exemplifies the power of 3D total scattering analysis for the combined structure determination of average and real structure of MOFs, thereby providing essential information for tuning distribution of species, defects and disorder towards finer control over their complex emergent properties [3].

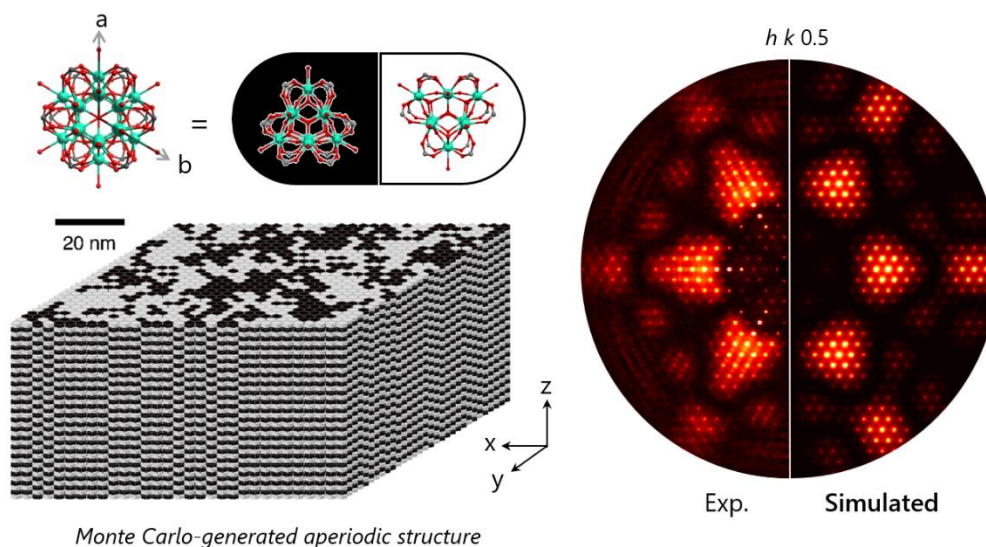


Figure 1. Simulated realistic distribution of cluster orientations in the disordered UoB-100 (left), and resulting diffuse scattering pattern, side by side with the experimentally observed one (right).

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## Unlocking Thin Film Disorder: High-Energy Diffuse Scattering with CdTe HPC Detectors

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Diffuse scattering, though often weak, provides crucial insights into short-range order beyond intense Bragg reflections, profoundly impacting a material's macroscopic properties (e.g. electronic, optical, and mechanical).<sup>[1]</sup>

Hybrid Photon Counting (HPC) detectors address the challenge of simultaneously measuring weak diffuse scattering and strong Bragg diffraction. They offer noise-free detection and high count rate capabilities by rapidly counting individual X-ray photons. This removes electrical noise from the data and enables the accurate measurement of weak diffuse data while maintaining precision for strong reflections. Furthermore, energy thresholds suppress interference from X-ray fluorescence or cosmic radiation.<sup>[2]</sup>

The hybrid design of these detectors allows choices for sensor materials. While silicon sensors are efficient for low to medium X-ray energies, their quantum efficiency diminishes above 15 keV. In contrast, CdTe sensors available for DECTRIS HPC detectors maintain high quantum efficiency up to 100 keV (Figure 1b).<sup>[2]</sup>

Here we show that a CdTe-based area detector can accurately measure diffuse scattering from crystalline thin films, enabling three-dimensional difference pair distribution function (3D- $\Delta$ PDF) interpretation previously limited to single crystals. For this experiment 74 keV (0.17 Å) X-ray radiation was scattered from PbTiO<sub>3</sub>/SrTiO<sub>3</sub> multilayer on SrTiO<sub>3</sub> using an ultra-small angle for grazing incidence diffraction (GID). High energy enables full coverage of reciprocal space up to a resolution of  $(2\sin(\theta)/\lambda) = 2.2 \text{ \AA}^{-1}$  and enables a geometry that reduces reflection smearing compared to medium energy-GID (Figure 1a). The resulting high-quality 3D- $\Delta$ PDF allows quantitative analysis of the disorder patterns in the PbTiO<sub>3</sub> layers.<sup>[3]</sup>

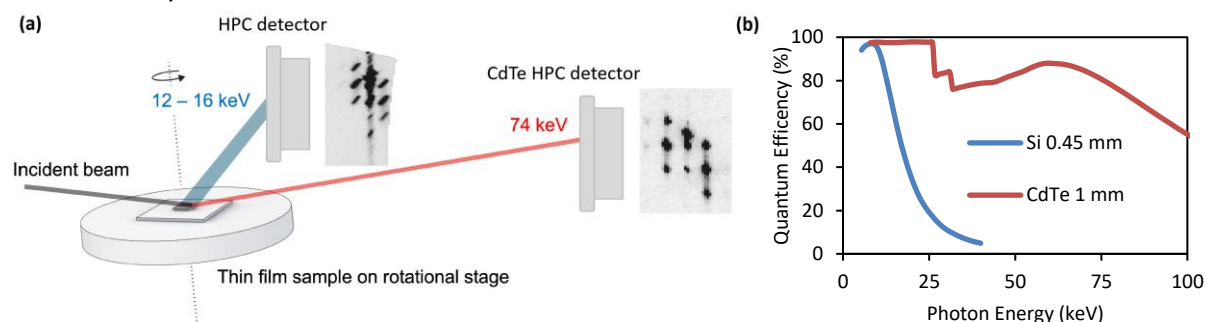


Figure 3- (a) Experimental setup for grazing incidence X-ray scattering, comparing medium-energy GID (blue) with high-energy GID (red). Detector images highlight how the high-energy setup reduces smearing around the 0 3 2 reflection. (b) Comparison of the quantum efficiency of a Si and a CdTe sensor as a function of photon energy.

By combining excellent dynamic range with modern sensor materials, HPC detectors are transforming our ability to comprehensively characterize materials. This capability is crucial for advancing our understanding of material properties and for guiding the design of next-generation functional materials where subtle structural details dictate performance.

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## Unveiling Magnetic Anisotropy in Layered Vanadyl Phosphates $\text{Ni}(\text{VO})_2(\text{PO}_4)_2 \cdot 4 \text{H}_2\text{O}$ and $\text{Co}(\text{VO})_2(\text{PO}_4)_2 \cdot 4 \text{H}_2\text{O}$ via Synergistic Magnetic, DFT+U Electronic Structure and Experimental Charge Density Studies

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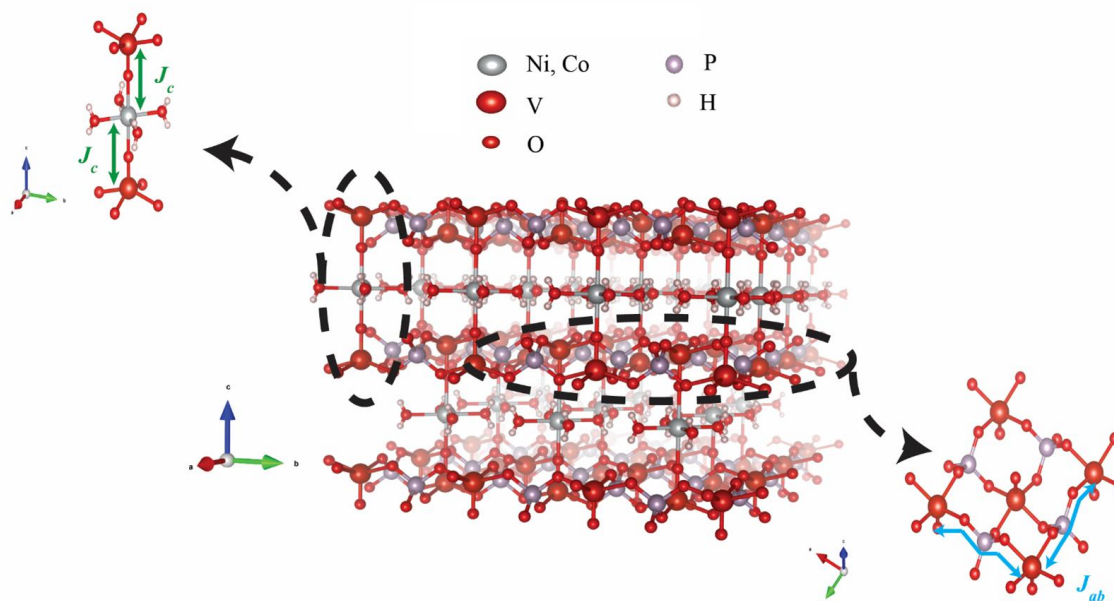
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2D layered vanadyl phosphates and their metal-intercalated derivatives have long attracted interest due to their catalytic, optical, and magnetic properties [1]. When intercalated with 3d transition metals, they serve as model systems for studying geometrical frustration, low-dimensional magnetism, and anisotropy. This work focuses on two isostructural tetragonal compounds,  $\text{Ni}(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$  and  $\text{Co}(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$  (space group  $I4/m$ ), comprising  $\text{V}^{4+}$  square pyramids connected via phosphate tetrahedra into layers in the  $ab$ -plane. These layers are linked along  $c$  by linear  $\text{V}=\text{O}-\text{M}-\text{O}=\text{V}$  ( $\text{M} = \text{Ni}^{2+}, \text{Co}^{2+}$ ) trimers, with  $\text{M}$  in octahedral  $\text{MO}_2(\text{H}_2\text{O})_4$  coordination (Figure 1).

Earlier models proposed bulk ferromagnetic coupling via an isotropic trimer spin Hamiltonian, assuming orthogonal  $e_g$  d-orbitals [2]. However, inverse susceptibility data suggest antiferromagnetic interactions. To clarify this, we combined oriented magnetic measurements on single crystals, DFT+U calculations, and X-ray charge density analysis.

Magnetic susceptibility measurements reveal anisotropic behavior: ferromagnetic along  $c$ , antiferromagnetic within the  $ab$ -plane, with partial moment cancellation. Long-range ordering emerges at 4 K, as confirmed by heat capacity data, with dominant low-dimensional antiferromagnetic correlations preceding 3D ordering.

Our interpretation of the exchange mechanisms is complemented by DFT+U calculations using CP2K code [3] and X-ray charge density measurements at 100 K, analyzed via Multipole Modelling (WINXD2024) [4], with a two-fold purpose of chemical bonding analysis and as comparison with theoretical transition metal d-orbital populations.



Layered structure of  $M(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$  compounds, showing trimer linker motifs (upper right) and Vanadyl phosphate layers (lower right), with magnetic super-exchange interaction pathways (green and blue arrows indicating interplane and intraplane pathways respectively)

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# An all-order phonon approach to thermal diffuse scattering

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In scattering experiments, phonons manifest themselves as Thermal Diffuse Scattering (TDS). Recent research has focused on phonons due to their role in various properties. This includes interactions like phonon-electron coupling in superconductivity and phonon-spin coupling, which finds application in spintronics, among other significant interactions. Understanding phonons and detecting phonon anomalies in materials is crucial in determining the material properties and their phase stabilities. Phonons are particularly important in elastic properties, with applications spanning from geology, where they aid in discerning planetary composition and temperature through the analysis of seismological wave propagation, to research in quantum phase transitions exploring their formation in crystals and interaction with other quasi-particles [1]. However, regular TDS, predominantly from acoustic phonon modes, often masks anomalies in phonons. While software exists for one or two-phonon processes, higher-order contributions are significant in certain systems. We are currently developing software capable of describing these higher-order contributions.

TDS arises from the scattering of X-rays by phonons and is present in all crystals. It contains valuable insights into phonon dispersion relations and the crystal elastic properties. Moreover, in many crystals static displacements give rise to intensity around the Bragg peaks which is very similar in shape to TDS, and thus can also be efficiently modelled using a similar approach. Currently, there are several programs available for modelling TDS, such as TDS2EL [2] and AB2TDS [3], however they have some limitations. In particular, TDS2EL allows to extract elastic constants from the TDS, but it can only model limited regions near Bragg peaks, while AB2TDS can cover all reciprocal space, but it utilizes single or two-phonon scattering approximations. In this work we propose a method to derive joint atomic displacement parameters which are used in conjunction with YELL [4] to model and fit real-space 3D- $\Delta$ PDF TDS signals efficiently. This approach avoids the need for large real-space models and offers good computational efficiency. Joint atomic displacement parameters are calculated based on the crystal's dynamical matrix, which can be derived using various methods, including universal potentials [5], DFT-based [6] approaches, or, in an approximated fashion, from the elastic constants of the material.

Our objective is to develop user-friendly software capable of describing TDS and TDS-like static disorder. Our approach offers faster computation compared to existing software and will be a valuable tool in the suite of 3D- $\Delta$ PDF software. It will facilitate the extraction of elastic constants from diverse materials and has the potential to be extended to extracting the portion of dynamical matrix responsible for high-amplitude soft phonons.

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## Structural Evolution of $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$ Solid Solution During Reductive Exsolution of Pt

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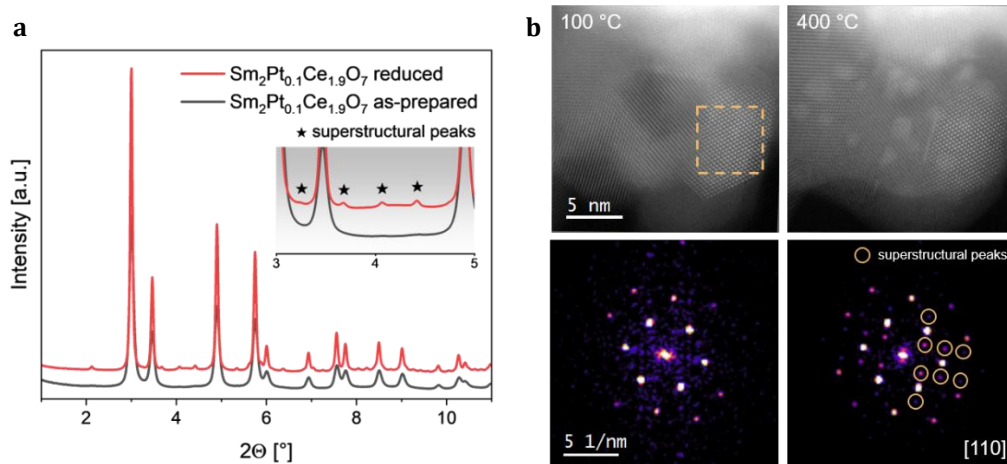
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Exsolution is a promising approach for the synthesis of supported nanoparticle catalysts that maintain stable catalytic activity under harsh reaction conditions — such as dry reforming of methane (DRM) — in contrast to catalysts prepared by conventional approaches, such as impregnation.<sup>1</sup> The enhanced stability of exsolved catalysts is commonly attributed to the stronger interaction between the support and the highly dispersed metallic nanoparticles (NPs) (anchoring of the exsolved NPs), arising during the reductive treatment of the initially doped host oxide solid solution.<sup>1</sup> In this study, we have developed catalysts for DRM by exsolution of Pt NPs from  $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$  solid solutions synthesized via a sol-gel method. To gain a deeper understanding of the exsolution mechanism, we employed synchrotron X-ray powder diffraction (XRD), pair distribution function (PDF) analysis of X-ray total scattering data, and in-situ scanning transmission electron microscopy (STEM) to characterize the structural and morphological changes that  $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$  undergoes during the exsolution process. Our findings show that Pt is initially incorporated into the oxide structure, forming a random fluorite-type (*Fm-3m*) solid solution ( $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$ ) (Figure 1a). Upon a reductive treatment, Pt NPs of  $\approx 2$  nm in size (Figure 1b) emerged on the surface of the host oxide, while the host undergoes a structural transformation into a C-type (*Ia-3*) structure. This C-type structure is a superstructure of the fluorite phase, distinguished by the ordering of oxygen vacancies and displacement of cations from the initial fluorite lattice positions.<sup>2</sup> The results presented in this study provide mechanistic insights into the reductive exsolution from ceria-based materials, highlighting a relationship between structural changes in the host oxide and the formation of exsolved NPs.



**Figure 1.** (a) XRD patterns of as-prepared fluorite-type  $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$  vs. reduced C-type  $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$ , (b) HAADF STEM images of  $\text{Sm}_2\text{Pt}_{0.1}\text{Ce}_{1.9}\text{O}_7$  at 100 °C vs. 400 °C with corresponding FFT patterns of a host oxide particle (in the dashed square) oriented along [110] zone axis.

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## Hydrogen storage in ice matrices at high pressure

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Hydrogen hydrates are promising functional materials for clean energy storage and offer alternative to the current cryo-compressed hydrogen storage technology, insuring low production and operational costs, environmentally benign nature, and lower risk of flammability. Hydrogen hydrate clathrate sII phase transitions into to the so-called “filled ice” forms above 0.8 GPa. In filled ice, the water frame assumes one of the known ice phases, and hydrogen occupies definite positions in the ice channels. Up to ~3 GPa, five different phases have been reported ( $C_{-1}$ ,  $C_0$ ,  $C_1$ ,  $C_1'$ , and  $C_2$  respectively), with increasing hydrogen-to-water ratio [1-2]. Recently, a new  $C_3$  phase with a hydrogen-to-water ratio of 2:1[2] forming above 40 GPa, upon laser heating (~1200 K), and being stable up to 90 GPa, has also been observed.

It has been shown that the  $C_2$ -form of hydrogen hydrate ( $H_2O \cdot H_2 / D_2O \cdot D_2$ ), which is constituted by an ice  $I_c$  skeleton, transforms into pure cubic ice  $I_c$  releasing molecular hydrogen upon decompression at 100 K [3]. However, the mechanism and kinetics of  $C_2$  hydrogen loss is not well-defined. It was suggested to progress through sample amorphization, though no evidence of an amorphous intermediate state was observed by neutron diffraction. We have recently determined, via high-pressure neutron powder diffraction experiments, that the unit cell volume of the  $C_2$  phase-produced in a Paris-Edinburgh (PE) cell at 3 GPa, and then recovered at ambient pressure and 78 K - continuously decreases upon heating above 100 K at ambient pressure. This indicates, at least partial, controlled hydrogen release without loss of crystallinity up to 130 K and the capability of  $C_2$  to store hydrogen up to 100 K at ambient pressure. Additionally, we present insights into structural deformation, phase boundaries, hydrogen content and mechanisms of formation of  $C_2$  under extreme pressure and/or low-temperature conditions. [4].

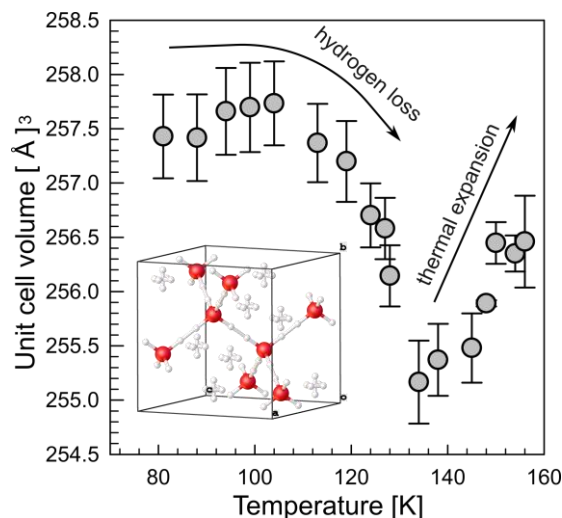


Figure 4- Unit cell volume variation during thermal decomposition of  $C_2$  hydrogen hydrate tracked with neutron powder diffraction ( $D_{20}$  at ILL). Inset: contents of the unit cell of  $C_2$  (oxygen in red)

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## Structure determination from complex powder mixtures

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The search for novel material increasingly employs the use of combinatorial synthesis. Simultaneously, structure solution from powder diffraction data has become a more mature field. However, structure solution usually requires single phase diffraction patterns [1], while combinatorial synthesis typically yields complex diffraction patterns of mixtures. So far, only serial rotation electron diffraction [2] offers a good way to structure determination in such cases.

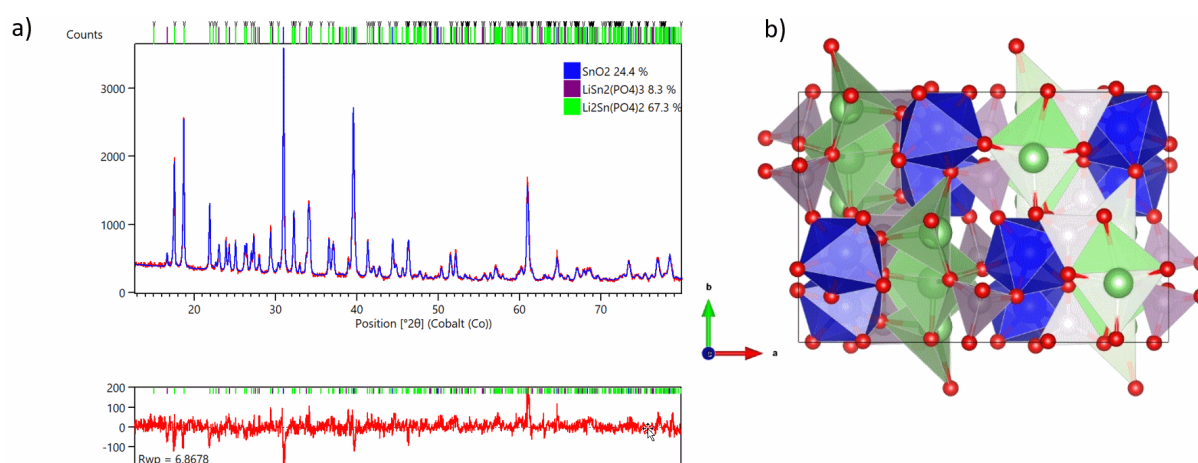


Figure 5 (a) Rietveld quantification and (b) crystal structure of the new ionic conductor  $\text{Li}_2\text{Sn}(\text{PO}_4)_2$

We present an alternative way to obtain structure solutions from complex mixtures where we deconvolute the various contributions from different phases and solve these structures individually. This approach was first used during the exploration of new hydrates and layered materials [3, 4] using powder diffraction data of mixture data. Finally, it enabled us to report 2 new candidates,  $\text{A}_2\text{Sn}(\text{PO}_4)_2$  ( $\text{A} = \text{Li}, \text{Na}$ ), for battery electrodes which were found during our investigation of the system  $\text{Li}/\text{Na}-\text{Sn}-\text{P}-\text{O}$  and were solved from 5-minute scans on an Aeris compact XRD. Both constitute a new type with in the  $\text{A}_2\text{M}(\text{PO}_4)_2$  series ( $\text{A} = \text{Alkali ion}, \text{M} = \text{Zr}, \text{Ti}, \text{Sn}$ ). The accuracy of the structure solution has been verified by DFT calculations.

The reported method unlocks the full potential of powder X-ray diffraction for structure determination in combinatorial chemistry.

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[3] G. Nénert, *Powder Diffraction* **2023**, 38 (3), 180-184, DOI: <https://doi.org/10.1017/S0885715623000301>

[4] G. Nénert, M. Avdeev ; unpublished.

## Control of liquid phase separation as a template for biomolecular self-assembly for industrial and biomedical applications

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As biomedical and biomaterial development accelerates and more complex systems are investigated and designed, there has been even more of a focus on battling degenerative disorders and diseases in our society.(1) Recently, Liquid-liquid phase separation (LLPS), already an interesting phenomenon that underpins many processes in the natural world and in our very bodies, has emerged as a potential platform to understand these disorders as well as template new materials and their intermediates for treatment.(2,3) Peptide mediated LLPS specifically has attracted much attention for its complex role in many disease (and treatment) pathways, as well as a platform for controlling crystallization for pharmaceutical compounds and crystals.(4) In this work we use the LLPS formation and growth pathways of oligocarbamates, peptide-like sequence defined synthetic polymers, as proof of concept for directing crystallization and stabilization of intermediate phases via ternary solution systems. Using *in-situ* coupled optical microscopy and Raman micro-spectroscopy, we monitor the evolution of sessile-drop evaporation driven LLPS and the formation of stable intermediate phases from solution. These intermediate phases are then characterized via AFM, OM and Raman micro-spectroscopy. This initial work is then used to guide the exploration of ternary-phase LLPS of two industrially and biomedically relevant peptide analogues: aspartame and kyotorphin. Formation pathways of intermediates are explored for fundamental interest and potential direct pharmaceutical and biomaterial applications.

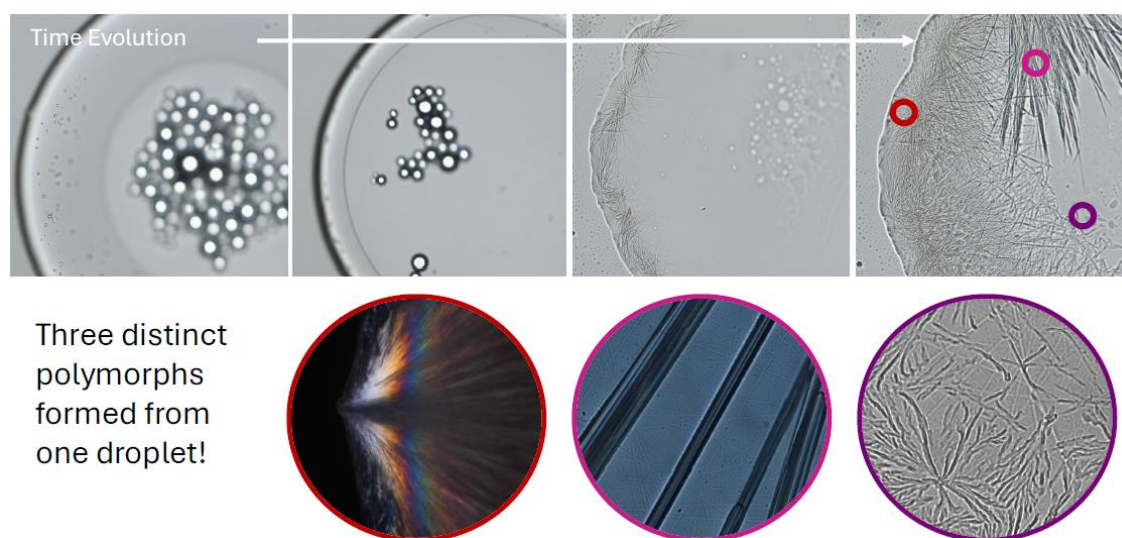


Figure 6- Time evolution of a complex, multicompartiment liquid droplet formed by liquid phase separation of Aspartame solutions showing eventual assembly and crystallization of multiple different crystalline forms (measured by Raman Spectroscopy, not shown). Colored rings correspond to highlighted ex-situ optical microscopy images of three separate forms of aspartame formed from the droplet.

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- (2) J. Berry; C. P. Brangwynne; M. Haataja et al., Rep. Prog. Phys. **2018**, 81 046601
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- (4) R. Chang; C. Yua; P. Zhou; R. Xing; X. Yan, Acc. Chem. Res. **2024**, 57,289–301

## The CaSO<sub>4</sub>-antibiotic system: Structural insights into the uptake and release mechanisms for infection treatment

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The discovery and development of new materials are crucial for overcoming the existing challenges in infection management, particularly in orthopedic and trauma surgery.<sup>1</sup> Local antibiotic therapy enables the delivery of antibiotics directly to bone and joint infections, while minimizing systemic toxicity.<sup>2</sup> Calcium sulfate (CaSO<sub>4</sub>) has gained attention as a promising osteoconductive carrier for antibiotics, such as vancomycin,<sup>2</sup> ceftriaxone,<sup>3</sup> and tobramycin<sup>4</sup> due to its biocompatibility and biodegradable properties. This study aims to investigate the molecular interactions and controlled uptake mechanisms of antibiotic-loaded CaSO<sub>4</sub> carriers.

We employed powder X-ray diffraction (PXRD) as the primary technique for in-situ kinetic studies of drug-carrier interactions at the molecular level. PXRD was used to track in real-time the polymorphic transition from hemihydrate to gypsum,<sup>5</sup> a process intrinsically linked to the hydration state of the CaSO<sub>4</sub> matrix loaded with various antibiotics (Fig. 1). Kinetic analysis revealed distinct transformation rates:  $0.040 \pm 0.015 \text{ min}^{-1}$  for CaSO<sub>4</sub>\_Ceftriaxone,  $0.045 \pm 0.005 \text{ min}^{-1}$  for CaSO<sub>4</sub>\_Vancomycin, and  $0.002 \pm 5 \times 10^{-4} \text{ min}^{-1}$  for CaSO<sub>4</sub>\_Tobramycin. Understanding of drug-carrier interactions is supporting the advancement of local antibiotic delivery, improving infection management and clinical outcomes in orthopaedic and trauma surgery.

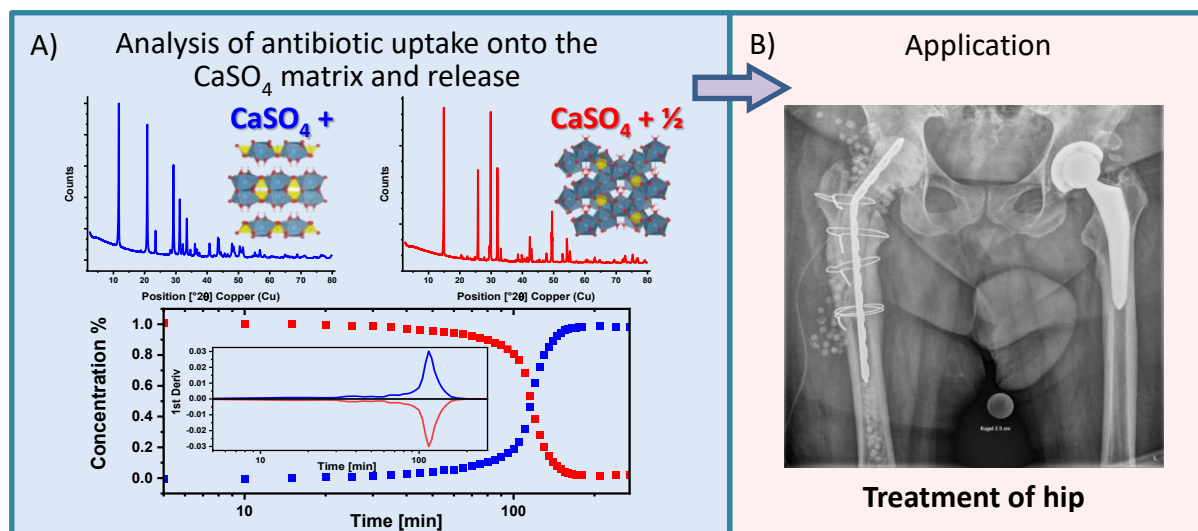


Fig. 1: Summary of analysis and application of the studied materials

### References:

- [1] Gramlich, Y., T. Johnson, M. Kemmerer, G. Walter, R. Hoffmann and A. Klug (2020), *Knee Surg. Sports Traumatol. Arthrosc.* 28(9): 2823-2834.
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## ***pgtrainer* : a classroom tool and 3D models for teaching point group symmetry**

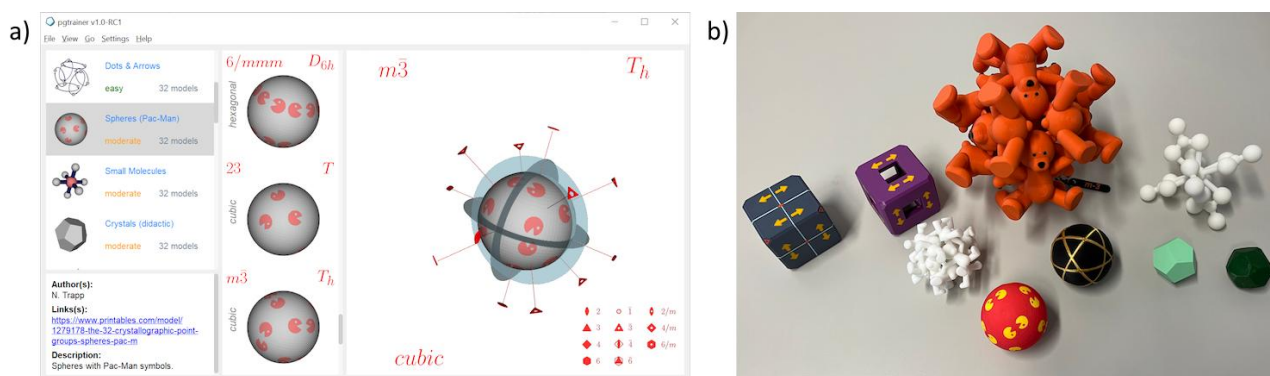
Dr. Michael Wörle [1], Michael Solar [1] and Dr. Nils Trapp [1]

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*pgtrainer* is a simple viewer program designed to assist with teaching point group symmetries, specifically the 32 crystal classes. It comes bundled with hundreds of different 3D models arranged in themed sets, such as crystal shapes, molecules or objects from daily life, with the intention of lowering the barriers for self study. The program has a simple & uncluttered interface, making it suitable for both projection in a lecture setting and practicing at home. Included models can be downloaded individually, and most are suitable for 3D printing.[1,2]

Models can be navigated by mouse, keyboard or presenter, and rotated/scaled/moved manually or automatically. Point group symmetry elements can be projected on the models. The user interface and displayed information are configurable and can be controlled with hotkey commands. This is a work in progress, i.e. more features will be added to the program. Installers for Windows and MacOS are available to download.[3]



**Figure 7-** Screenshot of the main *pgtrainer* program window with all GUI elements activated (a) and physical models representing point group  $m\bar{3}$  (b). White models were produced by an online 3D printing service (resin), colored models were printed on a hobby-level FDM printer.

Implementing more models into the program is relatively easy if they exist in .stl or .obj format. If you have your own and are interested in sharing them under a free license, please get in touch with the authors.

[1] <https://www.printables.com/@ntdesign/collections/2283402>

[2] <https://www.thingiverse.com/aarono/designs>

[3] <https://gitlab.ethz.ch/trappn/pgtrainer>

# The role of magma mixing in the petrogenesis of melilite-bearing nephelinite from southeast China

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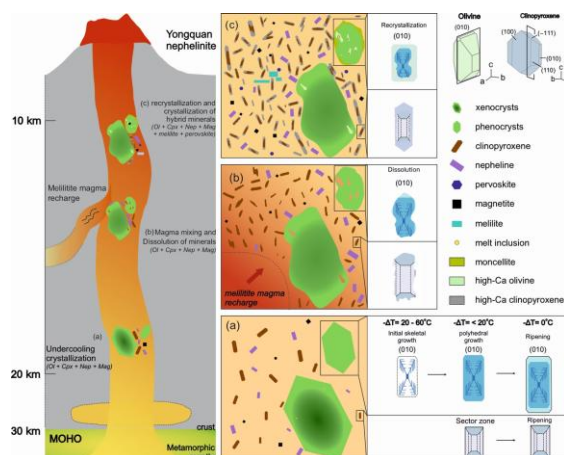
E-mail : yn.shi@email.cugb.edu.cn

Magma mixing is widely acknowledged as a prevalent magmatic mechanism [1], yet its significance in the formation of coexisting nephelinite and melilitite has frequently been overlooked. This oversight stems from the conventional assumption that nephelinite forms either through fractional crystallization from melilitite or directly sources from the mantle and rapidly traverse the crust [2, 3]. To bridge this knowledge gap, we provide a comprehensive petrological analysis of melilite-bearing nephelinite in Southeast China, which serves as a compositionally transitional facies between nephelinite and melilitite. This lava exhibits a distinctive mineral assemblage, including olivine, nepheline, clinopyroxene, titanomagnetite, melilitite, perovskite, monticellite, cancrinite, and sodalite—a combination first documented in nephelinitic lava flows. Crystals within this assemblage commonly display disequilibrium textures and intricate zoning patterns. Based on mineral textures and coexisting mineral phases, we infer that the unique mineral assemblage in the Yongquan melilite-bearing nephelinite results from the mixing of pre-existing nephelinitic magma with a recharged melilititic magma (Figure 1). Thermodynamic calculations outline a two-stage petrogenetic process for this rock type. The initial stage involved the crystallization of olivine-nephelinite melt at depths of approximately 18 km under moderate undercooling conditions. Subsequently, a hydrous (3.97–4.40 wt.% H<sub>2</sub>O), high-temperature (> 1060 °C) melilitite melt was emplaced into shallower (~11 km) magma conduits, initiating mixing with the resident magma. Thus, we conclude that mixing processes are pivotal in the petrogenesis of coexisting melilitite and nephelinite, rather than a straightforward evolution from melilitite magma. The groundmass zoning and phenocryst characteristics in nephelinite magmas reveal short-timescale dynamics, highlighting the necessity of integrating textural data with bulk-rock compositions for precise source signature interpretation.

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**Figure 1**—Schematic evolution model of magma mixing between nephelinite and melilitite magma resulting in the formation of the Yongquan nephelinite. (a) During rapid ascent, the low water content olivine nephelinitic melt underwent kinetically controlled crystallization at moderate-to-low undercooling, sequentially forming dendritic to polyhedral olivine phenocrysts with P-rich zoning, sector-zoned clinopyroxene, nepheline and magnetite at 1010–1050 °C. (b) The injection of a high-temperature, H<sub>2</sub>O-rich melilititic melt (> 1060 °C; 3.97–4.40 wt. % H<sub>2</sub>O) into magma conduits at ~11 km depth prompted mixing with the resident olivine-nephelinite melt. The resulting thermodynamic disequilibrium dissolved pre-existing olivine and clinopyroxene, producing resorption textures. (c) The ensuing disequilibrium promoted reactive growth of monticellite and high-Mg<sup>#</sup> clinopyroxene rims. Continued cooling then initiated fractional crystallization, sequentially precipitating diopside, melilitite, nepheline and perovskite.

## Collaborative Crystallography: Accelerating Discovery with DECTRIS CLOUD

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DECTRIS CLOUD is a web-based platform that reimagines how scientists collaborate, process data, and generate insight. Built around secure, real-time collaboration, the platform enables researchers to share datasets, software, and compute environments across global teams. Whether co-developing workflows or reviewing structural results, scientists can work together through browser-based access with no need for local setup or configuration.

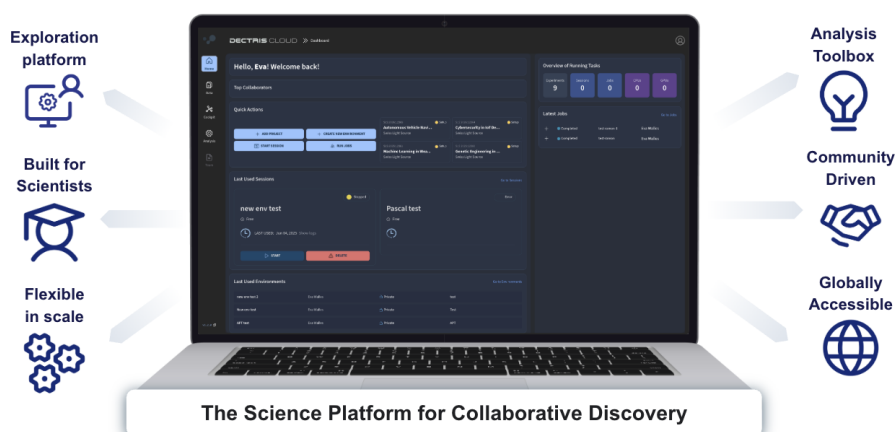


Figure 1- The DECTRIS CLOUD web application, an open platform for scientific discovery and real-time collaboration.

For crystallography, DECTRIS CLOUD brings together a comprehensive suite of community-curated software. These tools are available through ready-to-use, academic-licensed environments, while researchers can also create fully custom workspaces tailored to specific project needs with full control over the environment. The platform supports the entire crystallographic pipeline, from raw diffraction data to refined structures. Automated workflows support researchers through indexing, integration, structure solution, refinement, and analysis. Built-in virtual machines, Jupyter notebooks, visualization tools, and metadata curation features help document insights, support reproducibility, and strengthen data governance.

By eliminating computational barriers and reducing setup time, DECTRIS CLOUD allows scientists to concentrate on scientific challenges and discovery. The ability to collaborate effortlessly, adapt environments flexibly, and scale resources on demand makes it an ideal platform for advancing structural research.

# Crystal Growth and Characterization of Ytterbium-Based Silicate Materials

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The family of rare earth (RE) based silicate materials is quite vast, not only in terms of possible chemical compositions, but also in terms of the available crystal structures. In particular, the RE<sub>2</sub>SiO<sub>5</sub> (monosilicate), RE<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> (disilicate) families have attracted a lot of attention, mainly due to their polymorphic behavior as well as their peculiar physical and chemical properties. For example, the disilicate phase has at least seven known polymorphs that can be obtained based on the composition and temperature shown in figure 1 [1]. Meanwhile, the monosilicate system has two possible polymorphs referred in the literature as either X1 or X2. The X1 polymorph is always obtained with larger RE ions (La – Gd), however, in the case of smaller RE ions (Tb – Lu) X2 can be stabilized by using a relatively low calcination temperature between 900 and 1100 °C [2]. The natural abundance of the crystal structures as well as broad chemical composition ranges of rare-earth silicates led to an investigation of potential applications as either host materials for luminescence or for their scintillation properties. More recently, the silicates are being investigated as thermal barrier coating due to their thermal conductivity [3]. At the same time, their magnetic properties largely remain unexplored.

However, while promising the RE based silicates suffer significantly due to the lack high-quality single phase samples. The main reason for this is that the different phases, be it RE<sub>2</sub>SiO<sub>5</sub>, RE<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> or even the apatite ones are quite close in stability. As such, when preparing bulk samples, one often obtains a mixture of all or some of the phases. To further and unambiguously investigate the fundamental properties of the RE silicate materials, high-quality crystal samples are required. In this work we present the synthesis and crystal growth of Yb<sub>2</sub>SiO<sub>5</sub> and Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> using a laser diode optical floating zone furnace. We also investigate their crystal structure and quality by means of powder and single crystal X-ray diffraction as well as Laue diffraction.

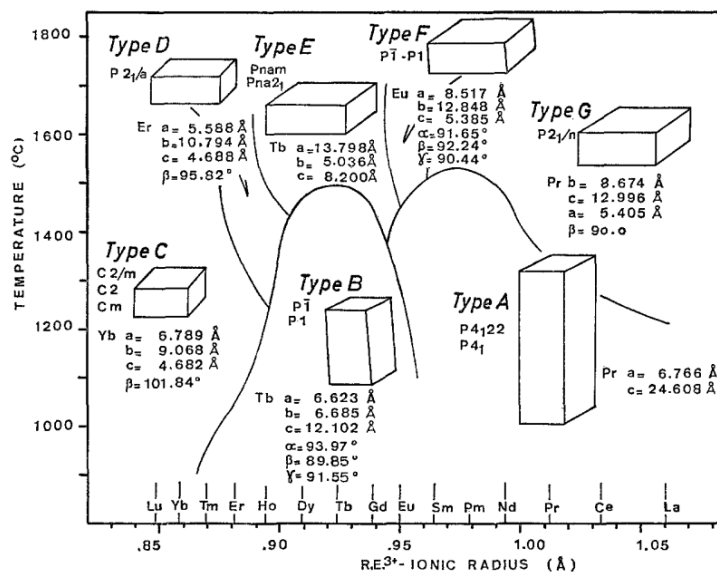


Figure 1- Graphical representations of the molecular structures of possible crystal structure of the rare earth disilicate compounds [1].

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## Effect of Deuteration on Glycine Crystallization: In Situ Raman Spectroscopy Insights into Non-Classical Nucleation and Polymorph Stability

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Crystallization from the liquid phase is a central process in materials synthesis, purification, and pharmaceutical formulation. A key challenge in this domain lies in understanding and controlling polymorphism—the ability of a compound to form multiple crystalline structures—which can significantly impact solubility, stability, and functionality of the final product. The effect of deuteration on crystallization behavior has been discussed in several occasions, because the use of deuterated solvents is essential for some characterization techniques. Some recent studies have reported the effect of deuteration on nucleation rates and polymorph outcomes, but the mechanisms underlying these differences remain elusive.

Glycine, a simple amino acid with three well-characterized polymorphs ( $\alpha$ ,  $\beta$ , and  $\gamma$ ), serves as a model system for investigating such effects. Under ambient conditions,  $\alpha$ -glycine typically forms in  $\text{H}_2\text{O}$ . In contrast, in  $\text{D}_2\text{O}$ , there are many literatures reporting the observation of  $\gamma$ -glycine—thermodynamically the most stable polymorph. However, some also reported no difference between  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$ . The discrepancies in literature motivated us to explore the effect of isotopic substitution on glycine polymorphs by using in situ Raman spectroscopy as a main tool.

In this work, we combined Single Crystal Nucleation Spectroscopy (SCNS) [1,2] and bulk crystallization characterization methods. SCNS enables one to monitor the Raman spectral evolution of polymorphic transitions at the single crystallization level. Our results show that in both  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$ , glycine undergoes a non-classical crystallization process: formation of prenucleation aggregates leads first to  $\beta$ -glycine, which rapidly transforms into  $\alpha$ -glycine. While a slight longer stability of  $\beta$ -glycine was observed in  $\text{D}_2\text{O}$ ,  $\gamma$ -polymorph was never observed. To compare the two systems at bulk crystallization level, we performed the measurement of crystallization induction time at 20 °C. Using the histogram of induction time, the nucleation rate and critical nucleus size were extracted. These values were, however, found similar between  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$ , with about three times slower nucleation rate in  $\text{D}_2\text{O}$ . We characterized the polymorph of glycine crystals formed in the vials used for induction time measurement. Only  $\alpha$ -polymorph was observed.

The puzzle of searching  $\gamma$ -polymorph was solved when we widened the crystallization condition further: crystallization from high degree of supersaturation ( $SS > 2.0$ ) or crystallization at low temperature. These conditions were achieved by either rapid solvent evaporation or cooling. Rapid solvent evaporation revealed that  $\gamma$ -glycine formed only from  $\text{D}_2\text{O}$  and not in  $\text{H}_2\text{O}$ . Under rapid cooling conditions, it was found that  $\gamma$ -polymorph appeared in both  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$ . Remarkably, the stability of  $\beta$ -glycine in  $\text{D}_2\text{O}$  appeared higher and it persisted for longer than 30 min in many conditions. DSC measurements confirmed the enhanced thermal stability of the deuterated glycine compared to glycine.

Collectively, we conclude that major effect of deuteration in the glycine crystallization is on the stability of  $\beta$ -glycine, which increases the probability of forming  $\gamma$ -polymorph in  $\text{D}_2\text{O}$ . The effect of deuteration at the molecular level as well as the microscopic picture of how polymorph stability is altered will be discussed. This work contributes to the broader effort of rationally controlling polymorphism in molecular solids.

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## High Pressure Research at Swiss Neutron Source

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The Swiss neutron source SINQ at Paul Scherrer Institute has recently undergone an extensive upgrade improving the versatility of several instruments as well as increased neutron flux. The increased performance opens up more opportunities for advanced-sample-environment research, such as experiments involving high pressure. In this contribution, we will present the current status of high-pressure sample environment at SINQ and will discuss our future plans.

[1] <https://www.psi.ch/en/lin/high-pressure-experiments>

## How Different Can Water Be?

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The distribution of O-H bond lengths in water molecules within crystalline hydrates reported in the Cambridge Structural Database (CSD) demonstrates a significant discrepancy between the datasets of structures measured using X-ray diffraction, and those determined by neutron diffraction. While neutron structures exhibit a mean O-H bond length of  $0.959 \text{ \AA} \pm 0.033 \text{ \AA}$ , the distribution of X-ray datasets shows an artificially shortened mean covalent bond length ( $0.861 \text{ \AA} \pm 0.070 \text{ \AA}$ ). The reason for the disagreement was found in the standard refinement model, the Independent Atom Model (IAM), which systematically underestimates X-H bond lengths, and in the use of a riding model with fixed hydrogen atom positions.[1] It was estimated that 180,000 of the 210,000 hydrate structures in the CSD may contain incorrect bond parameters and require re-refinement using Hirshfeld Atom Refinement (HAR).[2]

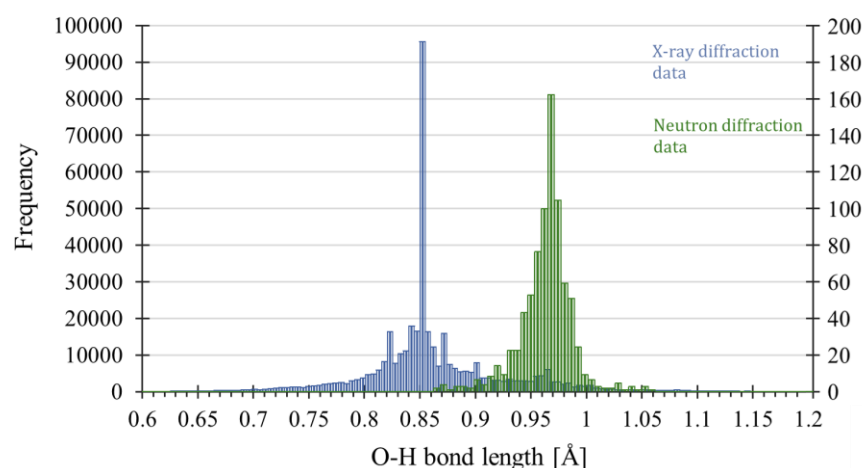


Figure 8- O-H bond length distribution of water in crystalline hydrates reported in the Cambridge Structural Database (CSD).

The presence of outliers in both datasets was attributed to the low energetic penalty associated with H-O-H bond angle deformations in isolated water molecules, as suggested by a potential energy scan in the gas phase. Thus, in the crystalline environment, such a small energy cost may be compensated by favorable intermolecular interactions, allowing for a broader distribution of bond angles.[3]

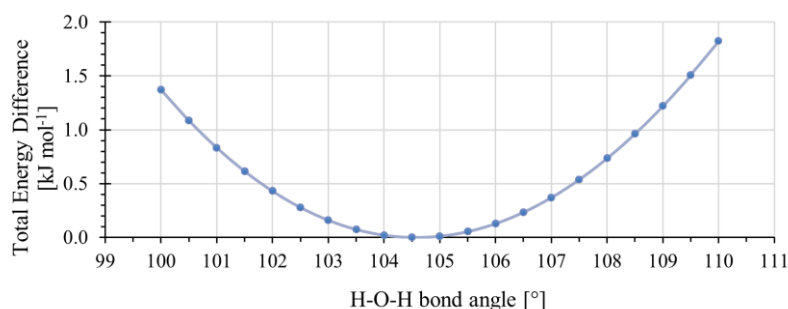


Figure 9- Potential energy scan of the H-O-H bond angle deformation in an isolated water molecule, calculated at CCSD/def2-QZVP.

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## Efficient Soft-Chemical Synthesis of Large van-der-Waals Crystals of the Room-Temperature Ferromagnet 1T-CrTe<sub>2</sub>

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We herein report on a fast and convenient soft-chemical synthesis approach towards large 1T-CrTe<sub>2</sub> van-der-Waals crystals. 1T-CrTe<sub>2</sub> is a metastable room-temperature ferromagnetic van-der-Waals material with a Curie temperature of  $T_C \sim 320$  K, which was first mentioned by Freitas *et al.* in 2015.[1] This compound is formed X-ray diffraction pure, with a complete conversion within just over 2 h from flux-grown LiCrTe<sub>2</sub> crystals [2] using diluted acids. Deintercalation of LiCrTe<sub>2</sub> using iodine, previously reported for the deintercalation of KCrTe<sub>2</sub> [1,3,4], was significantly slower and yielded partially deintercalated crystals. Due to the availability of high-quality single crystals, we have confirmed the crystal structure for the first time by single-crystal X-ray diffraction experiments. For the acid deintercalated 1T-CrTe<sub>2</sub> crystals, we find long-range ferromagnetic order with a Curie temperature of  $T_C = 318$  K. We further revealed the magnetic structure of 1T-CrTe<sub>2</sub> using low-temperature neutron powder diffraction experiments. X-ray diffraction experiments of postannealed crystals suggest a thermal stability of 1T-CrTe<sub>2</sub> up to at least 100 °C. Our findings expand the synthesis methods for 1T-CrTe<sub>2</sub> crystals, which hold promise for integrated room-temperature spintronics applications. [5]

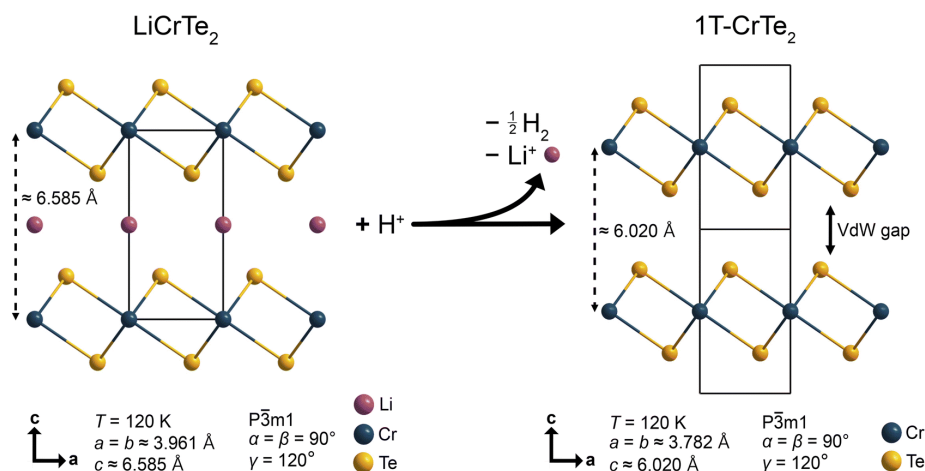


Figure 10: Acid-assisted synthesis of 1T-CrTe<sub>2</sub>: Scheme of the deintercalation reaction of LiCrTe<sub>2</sub> with an acid and the respective cell parameters of LiCrTe<sub>2</sub> and 1T-CrTe<sub>2</sub>.

- [1] Freitas, D.C.; Weht, R.; Sulpice, A.; Remenyi, G.; Strobel, P.; Gay, F.; Marcus, J.; Núñez-Regueiro, M; *Journal of Physics: Condensed Matter*, **2015**, *27* (17), 176002.  
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## The new PHOTON IV Detector and benefits of hard radiation

Tobias Dunaj (1), Martin Adam (1), Carsten Lenczyk (1), Anna Luebben (1) and Tobias Stürzer (1)

*Bruker AXS SE*

*Email: tobias.dunaj@bruker.com*

Single crystal structure determination from samples containing a certain number of heavy elements can severely suffer from absorption, even if relatively hard radiation Mo-K $\alpha$  radiation is applied. Modern X-ray sources (I $\mu$ S 3.0, I $\mu$ S DIAMOND II, METALJET MC) give access to harder Ag- or In-K $\alpha$  radiation. Harder radiation addresses absorption issues and additionally it provides better sample transmission, higher maximum resolution, and a very straight forward data reduction. These properties render Ag-K $\alpha$  radiation, particularly, ideal for advanced applications like charge density or high-pressure pressure studies or material science investigations on heavily absorbing samples in general. However, the benefit gained from the high energy radiation can be ironed out or even turned into the contrary if not properly reflected by the detector properties. Silicon-based X-ray detectors typically miss out two out of three X-ray photons reflecting the poor absorption capabilities of Silicon for the high energy X-ray photons. With the PHOTON IV HE, a photon-counting detector is now available, which perfectly matches the properties of hard X-ray radiation, yielding an unparalleled high quantum efficiency for Ag-radiation. Along several selected examples, we will demonstrate the benefits generated combining a hard radiation source with a PHOTON IV HE.

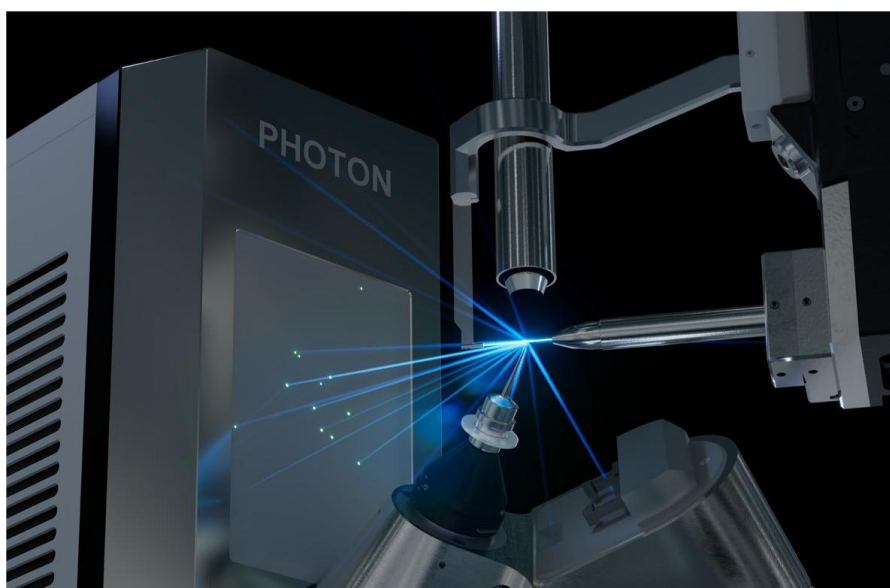


Figure 11- Artistic representations of X-ray scattering and data collection with the all new PHOTON IV X-ray detector.

## Agenda of the General Assembly 2025

### Swiss Society for Crystallography SGK/SSCr

Wednesday, 10.09.2025

EPFL – Bâtiment SV, Auditorium: SV 1717, SV, 1015 Ecublens, Lausanne, Switzerland

#### Agenda:

1. **Determination of the Quorum (Art 12, by-laws)**
2. **Proposition for acceptance of the minutes of the General Assembly 2024 (Basel)** (published in Newsletter No. 113)
3. **Reports**
  - a) Annual report of the President
  - b) Delegates to adhering bodies (IUCr, ECA, IOCG)
  - c) Annual financial statement (2024) and forecast 2025
  - d) Budget for next year (2026)
  - e) Vote on membership fees
4. **Elections**
  - a) Confirmation of the current board members
  - b) Nomination of new board members. To be submitted to the president 10 days prior to GA. Suggestion: Ekaterina Pomjakushina, PSI.
  - c) Nomination of new functions of board members. Suggestion: New Vice-President, Ekaterina Pomjakushina; new Treasurer, Pascal Schouwink.
  - d) Confirmation of SCNAT delegate
  - e) Election/Confirmation of the auditors
5. **Annual Meeting and General Assembly 2025: Decision on location and organizer.** Suggestion: St. Gallen, September 8-10, 2026, Bruno Silva and Antonia Neels.
6. **Discussion about future teaching initiatives of SSCr**
7. **Report on conferences 2026: CECAM, EPDIC and IUCr**
8. **Discussion about UNESCO Africa Initiative**
9. **Other motions of members and communications:** should be communicated to the president 10 days prior to the meeting.

## SSCr PhD Prize 2025

The Swiss Society for Crystallography awards the 2025 PhD Prize to Dr. Yevhenilia Kholina for her exceptional thesis, “Correlated disorder in Prussian Blue analogues: from understanding to control of the local structure.”

Her research, conducted at the Laboratory for Disordered Materials, Department of Materials, ETH Zurich, under the supervision of Prof. Arkadiy Simonov, combines advanced 3D $\Delta$ -PDF analysis and Monte Carlo simulations to reveal how correlated disorder influences material properties, even when chemical composition and average structure remain unchanged.

Dr. Kholina demonstrated how to control disorder using accessible synthesis parameters, enabling practical applications such as enhanced hydrogen storage and symmetry tuning. She also discovered hidden phase transitions detectable only through diffuse scattering.

We warmly congratulate Dr. Kholina on this achievement and look forward to her continued contributions to crystallography.

The award will be presented at the SSCr Annual Meeting in Lausanne, on September 10, at 11:10.

With its long-standing tradition in crystallography and structural science, the Swiss Society for Crystallography also maintains a tradition of awarding a prize for the best PhD thesis in the field.



## SSCr Travel Grants: awardees' reports

We congratulate Bang Joohee, Kai Röseler, Dan Stefanita, and Samira Baumann on their travel award and successful participation in international events.

### Report on Participation at the 2025 MRS Spring Meeting Seattle, USA, April 7–11, 2025 By Bang Joohee, ETH Zürich



I sincerely thank the Swiss Society for Crystallography (SGK/SSCr) for awarding me a travel grant to attend the 2025 MRS Spring Meeting in Seattle. With their generous support, I had the opportunity to deliver an oral presentation titled “Noninvasive Three-dimensional Mapping of Polar Skyrmion Structures with Atomic Resolution” in the session on Ferroic Materials and Heterostructures.

The conference served as an outstanding platform to share my expertise in advanced crystallography with leading researchers in oxide electronics. I presented the first noninvasive atomic-scale analysis of polar skyrmion domains in ferroelectric superlattices, achieved through diffuse

X-ray scattering analyzed with the 3D- $\Delta$ PDF method. This pioneering study demonstrated how high-quality, large-volume diffuse X-ray scattering data paired with  $\Delta$ PDF analysis can significantly advance the investigation of local order in single-crystalline thin films. Engaging discussions that followed the talk highlighted the potential of this approach to drive future progress in the structural characterization and application of topological thin film systems.

The SGK/SSCr travel grant played a crucial role in making this experience possible, covering key travel expenses and enabling my active participation. I am deeply appreciative of the society’s support in helping bridge advanced crystallographic techniques with condensed matter physics. I look forward to integrating the insights and connections gained from this meeting into my ongoing research.

### 33rd Annual Meeting of the German Crystallographic Society (DGK) 2025, Hannover, Germany, March 10- 13, 13.03.2025

*By Kai Röseler, University of Geneva*



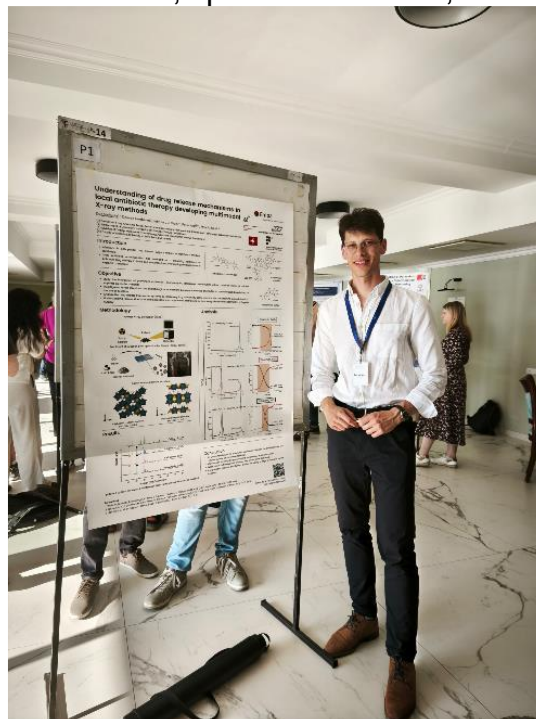
I am grateful to have received the travel award from the SSCr, which allowed me to attend the general annual meeting of the German crystallographic society (DGK) in Hannover. Participating in the DGK conference provided me with

valuable insights into the work of renowned crystallographers. Among the many excellent presentations, I found talks in a symposium on “Complex and Aperiodic Structures” especially impactful. Since my research, among others, involves the soft chemical synthesis of novel quantum materials, disorder and stacking faults are a common feature, for which I now have a clearer understanding of. Poster sessions and coffee breaks led to very interesting discussions, which inspired me to explore new ways of manipulating quantum systems, with the aim of discovering novel crystal structures. In addition to the insights during the discussions, the stimulating and welcoming atmosphere has led to sparking ideas for possible future collaborative efforts. While I remain deeply enthusiastic about the synthesis and characterization of quantum materials, I also greatly value the insights I gained into the many facets of crystallographic work. The conference concluded with a symposium on physical crystallography, where I had the pleasure of sharing the results of our recent publication of the acid assisted synthesis of  $\text{CrTe}_2$ , which was well attended. After getting to know the (mostly) German crystallographic community, I very much look forward to engaging with the SSCr community in September.

**Report for SSCr Travel Award 10th European Crystallography School, 22-27 June 2025, Ohrid, N. Macedonia  
By Dan Stefanita, Empa**

The 10<sup>th</sup> European Crystallography School, organized by the European Crystallographic Association (ECA), was a great opportunity to meet fellow researchers, students, and great speakers from around the world. The school was exceptionally well organized, featuring a diverse program

of lectures, poster sessions, virtual



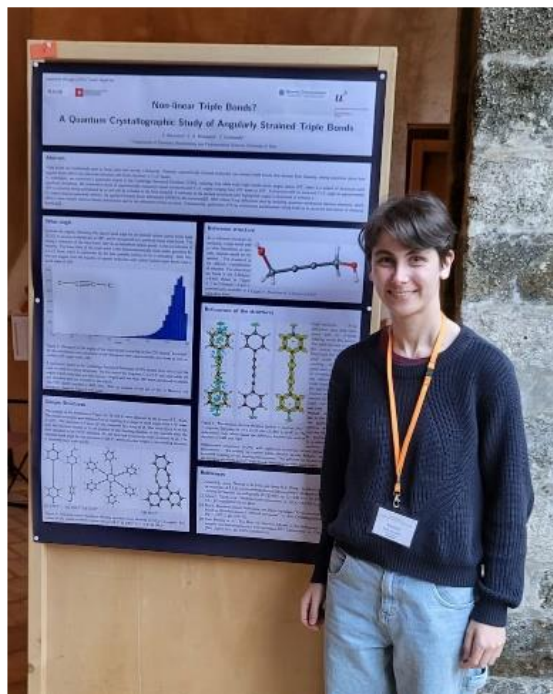
tours of synchrotron facilities, excursions, and hands-on workshops. I had the privilege of presenting my research work during the poster session, which facilitated valuable discussions, constructive feedback, and suggestions from both peers and experts. This helped me shape my current studies and inspired me for my future work.

Despite our different backgrounds, we had the opportunity to network and share common interests. I was very excited to exchange ideas and discuss different topics with the lecturers and other attendees. The school significantly deepened my understanding of the foundational aspects of the topic and encouraged me to explore innovative approaches in my research. One of the highlights for me was the practical workshop on EXPO software, which has equipped me with new skills that I am now applying to refine my own crystal structures.

Attending the European Crystallography School was a great and memorable experience. The diversity in the topics and classes made me understand how much we can learn and that we can always ask for help in our

community. I am grateful for the opportunity to participate and for the support provided by the SSCr Travel Grant. Special thanks go to the organizers, invited speakers, my supervisor Prof. A. Neels, and the SSCr for making this experience possible. I look forward to applying the knowledge and insights gained as I continue my research journey.

**Impressions from the International School of Crystallography  
Erice, Italy, May 30 to June 7, 2025, in  
By Samira Baumann, University of  
Bern**



I was very happy to attend the 61st course of the International School of

Crystallography on Quantum Crystallography, held from 30 May to 7 June, 2025, in Erice, Italy. It was a highly rewarding experience, both scientifically and personally. The parallel 60th course on electron crystallography provided a valuable opportunity for interdisciplinary exchange.

The school offered an intensive mix of lectures and hands-on workshops. Early lectures covered fundamental topics like direct and reciprocal space, structure solution and refinement, and basics of quantum crystallography. As the week progressed, more advanced topics such as bonding analysis were introduced. The workshops complemented the lectures by providing practical experience with a range of relevant software tools.

Coffee breaks and poster sessions, where I presented my own research about non-linear triple bonds, enabled engaging discussions with fellow participants about our research. Meeting students and young researchers from around the world was truly inspiring.

I'm very grateful to the Swiss Society of Crystallography for making my participation in the school possible and for supporting young scientists like me. The experience deepened my knowledge and helped me connect with a vibrant, international community. I would wholeheartedly recommend this school to anyone looking to strengthen their foundation in crystallography.

## Invited article: Memories of my relations with the Swiss Society for Crystallography

Hans Grimmer  
hans.grimmer@bluewin.ch



Having finished my research work for a PhD in mathematical physics at Edinburgh University in 1968, I joined the Battelle Advanced Studies Center in Geneva as a member of the group of Edgar Ascher [1]. He was a member of the Swiss Society for Crystallography (SSCr) from its founding in 1969. As crystallography grew out of mineralogy, the SSCr grew out of the Swiss Society of Mineralogy and Petrology (SSMP). Werner Nowacki, Professor of Crystallography at the University of Berne, felt that the interests of crystallographers were not adequately represented by the SSMP. He suggested the foundation of the SSCr and became its first president 1969-1972, followed by Edgar Ascher 1972-1975.

In Geneva, I collaborated also with two other researchers that had joined the SSCr already in its founding year 1969. One was Walter Bollmann, known for his work in transmission electron

microscopy (TEM). He was one of the first who observed dislocation lines in TEM micrographs. In order to interpret the dislocation networks that he observed in low-angle grain boundaries, he developed a general geometrical theory of crystalline interfaces [2]. Our collaboration was the starting point of my most successful research project.

The other was Hans Schmid, a physical chemist who worked on ferroelectric materials. In 1964 he grew single crystals of the boracite  $\text{Ni}_3\text{B}_7\text{O}_{13}\text{I}$ , the first material that was found to be simultaneously ferroelectric, (weakly) ferromagnetic and ferroelastic. Together with Ascher, he showed that in this boracite the spontaneous electric polarisation can be switched by a magnetic field and the spontaneous magnetisation by an electric field. In 1977 he moved to the Department of Inorganic, Analytic and Applied Chemistry of the University of Geneva, where he was full professor from 1978 until his retirement in 1996. From 1981 – 1984 he served the SSCr as vice-president and chairman of the section for crystal growth [3].

Hans Schmid asked me to help organizing the 2<sup>nd</sup> International Conference on Magnetolectric Interaction Phenomena in Crystals (MEIPIC-2), held in 1993 at the Centro Stefano Franscini, Monte Verità, Ascona. I found this a most stimulating experience.

When André Authier prepared Volume D of “International Tables for Crystallography”, dedicated to physical properties of crystals, he asked Hans Schmid to propose contributing authors. He suggested that I might support Andrey S. Borovik-Romanov writing the chapter on “Magnetic Properties”. We sent our manuscript to Authier in 1994. When all contributions had arrived, Volume D was published in 2003, six years after the death of Borovik-Romanov.

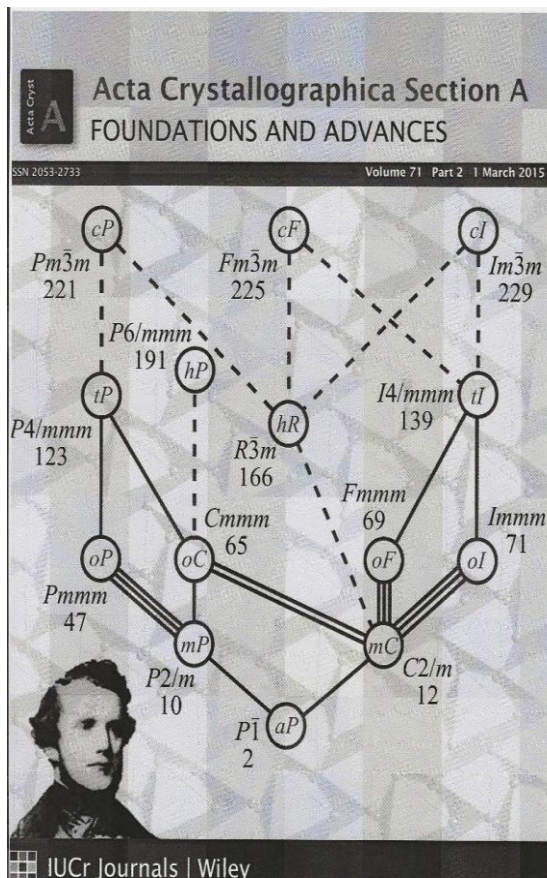
When Dieter Schwarzenbach became President of the SSCr in 1984, Howard Flack was Secretary of the SSCr and

started editing a Newsletter [4]. He edited Newsletters 1 to 25 during his time as Secretary from 1984-1990. Helen Stöckli-Evans edited Newsletters 26 to 33 during her time as Secretary from 1990-1993. Then she became President from 1993-1996 and Gervais Chapuis took over as Secretary. He was not interested in editing the Newsletter and delegated this task to Karin Cenzual (Newsletters 34-43). When Gervais Chapuis became President from 1996-1999, she continued this task until 1997. I edited the Newsletters 44 to 66 (1998 – 2005), 1999-2002 as President and 2002-2005 as Secretary of the SSCr. This was possible thanks to the generous support of my employer, the Paul Scherrer Institute, which printed and distributed the Newsletter at its costs.

In the paper «The History of Crystallography in Switzerland» [5] Volker Gramlich wrote the first three chapters and I the last “The Swiss Society for Crystallography”. The “History of Crystallography in Switzerland” was updated in [6].

In 2016 the SSCr organized the European Crystallographic Meeting ECM30 in Basel. Newsletter 96 contains a reprint of [6] and a survey of all the crystallographic research groups active in Switzerland. It contains 28 entries! The Newsletter was made available to the more than 900 participants of ECM30. The meeting was a great success, as described in Newsletter 97. On page 9 it shows “our long term members Hans Grimmer and Howard D. Flack” in lively discussion. It is a sad coincidence that the same Newsletter also contains the “Obituary Howard Flack” written by Radovan Černý

I am greatly indebted to Howard: A manuscript “Relations between the 14 Bravais types of lattices”, which I submitted in 2014 to Acta Cryst. A, was rejected as being trivial. Thanks to his suggestions, a revised version [7] appeared in the “Advances” section together with a comment by Howard Flack.



**Cover illustration:** Bravais described his complete set of space-filling lattices in 1850, but new insights into the hierarchical relationship between the Bravais lattices described in this issue [Grimmer (2015). *Acta Cryst. A* **71**, 143-149; see also Flack (2015). *Acta Cryst. A* **71**, 141-142] will give scientists powerful new tools in predicting new structures and understanding phase transitions, such as the magnetic ordering in haematite (shown as a backdrop). Image courtesy of K. M. Ø. Jensen, Columbia University.

The 2016 edition of Volume A of “International Tables for Crystallography” shows some of the results of [7] in its Section 3.1.4, written by Boris Gruber and myself.

I am most grateful to the SSCr and many of its members for the great support that I received on so many occasions.

#### References

- [1] H. Grimmer “In Memoriam Edgar Ascher” SGK/SSCr Newsletter 69 (2006) 13-14.
- [2] H. Grimmer “In Memoriam Walter Bollmann” SGK/SSCr Newsletter 77 (2009) 16-17.
- [3] H. Grimmer “In Memoriam Hans Schmid” SGK/SSCr Newsletter 93 (2015) 16-17.
- [4] E. Giannini “40 years of newsletter” SGK/SSCr Newsletter 113 (2025) 13-15.

[5] V. Gramlich, H. Grimmer "The history of crystallography in Switzerland" *Chimia* 55 (2001) 484-486.

[6] H. Grimmer "History of crystallography in Switzerland" *SPG Mitteilungen* 42 (2014) 24-27.  
[7] H. Grimmer, *Acta Cryst.* A71 (2015) 143-149.

## Minutes of the General Assembly 2024

Swiss Society for Crystallography SGK/SSCr

Friday, 12.09.2024, 12:40-13:30

Innovation Park Heggenheimermatt 167, 4123 Allschwill, Basel Switzerland

### Agenda:

10. **Determination of the Quorum (Art 12, by-laws)**
11. **Proposition for acceptance of the minutes of the General Assembly 2023 (Zürich)** (published in N112, pp 49-55)
12. **Proposition for changes in the by-laws**
13. **Reports**
  - a) Annual report
  - b) New incentives
  - c) Delegates to adhering bodies (IUCr, ECA, IOCG)
  - d) Annual financial statement (2022)
  - e) Budget for next year (2024)
14. **Elections**
  - a) Definition of chairperson for elections
  - b) Confirmation of the current board members
  - c) Change of presidency, proposition Simon Grabowsky (Bern)
  - d) Nomination of new board members. To be submitted to the president 10 days prior to GA.
  - e) Confirmation of SCNAT delegate
  - f) Election/Confirmation of the auditors
15. **Annual Meeting and General Assembly 2025: Decision on location and organizer**
16. **Other motions of members and communications:** should be communicated to the president 10 days prior to the meeting.

### Minutes:

#### 1- Quorum and formalities

The General Assembly was chaired by Pascal Schouwink, President.

The agenda was published in the SGK / SSCr Newsletter No. 112 (2024) page 29.

The secretary, Paula Abdala, ETH, was appointed as taker of the minutes.

With 29 members being present at this assembly, the necessary quorum of 10% (18) is reached to constitute a quorum (Art. 12).

We have 187 records of members in our database as of 05.09.2024.

They are grouped as:

- 11 Corporate members
- 161 personal members (F + S)
- 15 Honorary members

**New entries 2024:** 12

Note: Members who have not paid the annual fees for more than 3 years and who cannot be contacted can be removed from the database.

- 2- **Proposition for acceptance of the minutes of the General Assembly 2023, held:** 08.09.2023, University of Zürich (Irchel Campus) 13:15 h – 14:15 h

The General Assembly was chaired by Pascal Schouwink, President, 13:15 h – 14:15 h

The minutes have been published in Newsletter 112, August 2024. ([The SGK/SSCr Newsletter | Swiss Society for Crystallography \(SGK/SSCr\)](#))

The secretary, Paula Abdala, ETHZ, was appointed taker of the minutes.

Correction (updated on the online version):

The budget 2021 has been approved by the auditors B. Spingler and A. Neels

Replaced by

The financial report 2022 has been approved by the auditors B. Spingler and A. Neels

**Voting:** the minutes were approved unanimously, without abstentions.

### 3- Proposition for changes in the by-laws

#### Summary of the changes introduced:

- Introduction of both male and female form
- Change of domicile to Bern (avoiding outdated address information)
- Removal of the archive (no hardcopy documents kept, only a newsletter collection)
- Removal of a suggestion for the membership fee (which was anyway outdated)
- Flexibility in removing members upon not paying membership fee. Decision now with the board after more than two years.
- Simplification of the structure of sections in general, and specifically for the Section for Crystal Growth and Crystal Technology (SCT).
- Removal of passive board members (German: Beisitzer), only active roles:  
President, Vice-President, Secretary, Treasurer, Webmanager (not mandatory), Eventmanager (not mandatory)
- Automatic assignment of delegation seats to board members (if possible, otherwise replacement to be organized):
  - ✓ Secretary for IUCr: Secretary of SSCr (for a period of three years, not six)
  - ✓ General Assembly of IUCr: President and Vice-President
  - ✓ ECA Council: Vice-President

**Voting:** the changes in the by-laws were approved unanimously, without abstentions.

### 4- Activity report

The President, Pascal Schouwink, provided an overview of the key activities of the board of the SGK-SSCr in the past year.

-Mention to: Dieter Schwarzenbach 1936-2024, President SSCr 1984 – 1987, Obituaire on page 30-33, Newsletter 112

#### Travel grants and prizes

Travel support has been awarded to six young members for attending events in 2023, and there is encouragement to promote becoming an SSCr member and to apply. Note that PhDs and Postdocs under 35 years old are eligible to apply. The SSCr PhD prize is announced during this meeting.

#### Howard Flack Crystallographic Series

The Howard Flack Crystallographic Series in 2023 was a success, featuring the Local Order and Pair Distribution Function Analysis - Total Scattering and AI

approaches, by Simon Billinge. Series 2024 has been canceled. Proposals for topics for future series can be submitted to [swiss.crystallography@gmail.com](mailto:swiss.crystallography@gmail.com).

#### The SSCr Topical Workshop

As a satellite of this meeting, the SSCr Pair Distribution Function Analysis workshop was held. The workshop hosted 40 participants (59 registrations), and received SCNAT financial support. Speakers at the event were: Gwilherm Nénert – Malvern Panalytical; Michael Evans – Bruker; Ann-Christin Dippel – DESY; Alex Hannon – ISIS; Diana Piankova – ETH Zurich; Fernando Igoa – DESY.

#### National & International cooperation

ZSC update: Secured for 2024, the organizers should explore solutions to maintain beyond, i.e. 2026.

Erice powder diffraction school in 2024 (co-direction and teaching by board members)

BM01 summer school: participation of SSCr board members in organization and teaching

### **3c) Annual financial report**

Enrico Giannini (Treasurer) presents the closing of the financial year 2023 and the financial situation in 2024.

#### **Summary SGK Finances 2023**

	<b>CHF</b>
<b>Total 31.12.2022</b>	<b>46'170.27</b>
UBS account	46'391.46
Cash on hand	398.25
<b>Total 31.12.2023</b>	<b>46'789.71</b>
<hr/> <b>Balance</b>	<b>+ 619.44</b>

#### **Report of revisors:**

The budget 2023 has been approved by the auditors B. Spingler and A. Neels.



## SGK Financial Report 2023

### Income:

Membership dues:

Full members (various amounts due to debts)

52x40 + 2x50 + 2x60 + 1x70 + 15x80 + 7x120 + 1x160+ 1x378.29  
+ 1x400

5'348.29

Students 14x10 + 3x20 + 1x30

230.00

Companies 12x130 + 1x124.59

1'684.59

Total membership

**7'262.88**

Sponsorship

2'000.00

Subsidy SCNaT (2023)

9'801.75

Interests

157.65

**Total Income 19'222.28**

## SGK Financial Report 2023

### Expenses:

Membership dues to SCNat

1'057.00

Travel costs of IUCr/IOCG delegates

2'000.00

Annual Meeting

3'000.00

Topical Workshop of the SGK

2'881.38

IUCr satellite workshop

812.05

Travel Grants (including PhD prize)

5500.00

Howard Flack Lecture Series

1'484.35

Association to ECA

176.05

Printing and publishing costs (newsletter)

1'480.25

Bank expenses

211.76

**Total Expenses 18'602.84**

**Income – Expenses**

**+ 619.44**

### Cash on Hand - 2023:

**Status 31.12.2022**

**515.55**

Total Income

0.00

Total Expenses

117.30

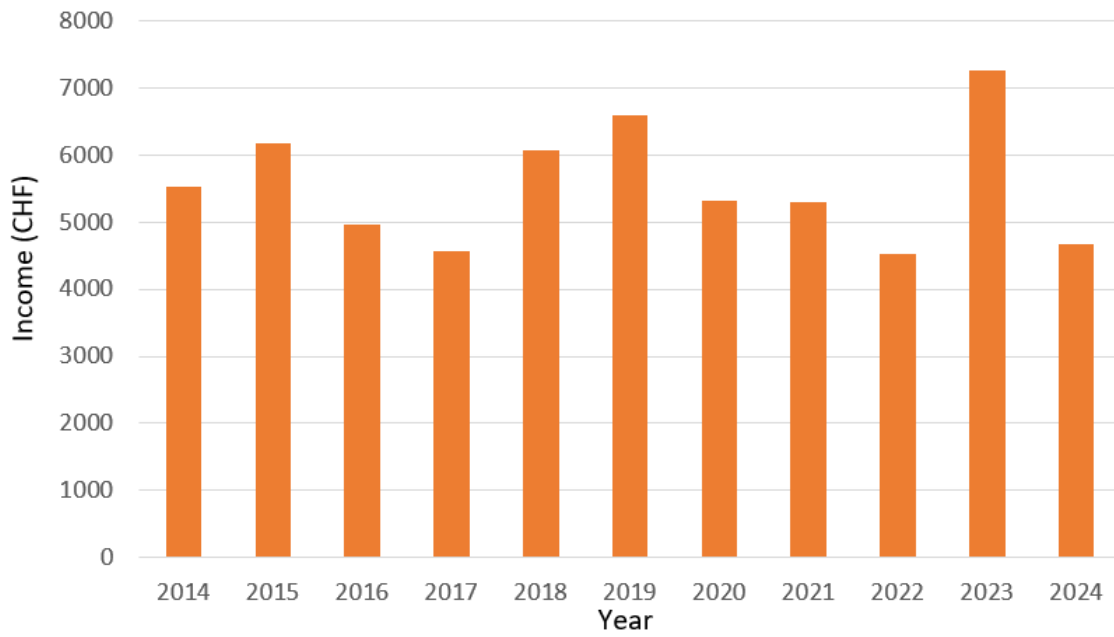
Starting Balance + Income – Expenses

398.25

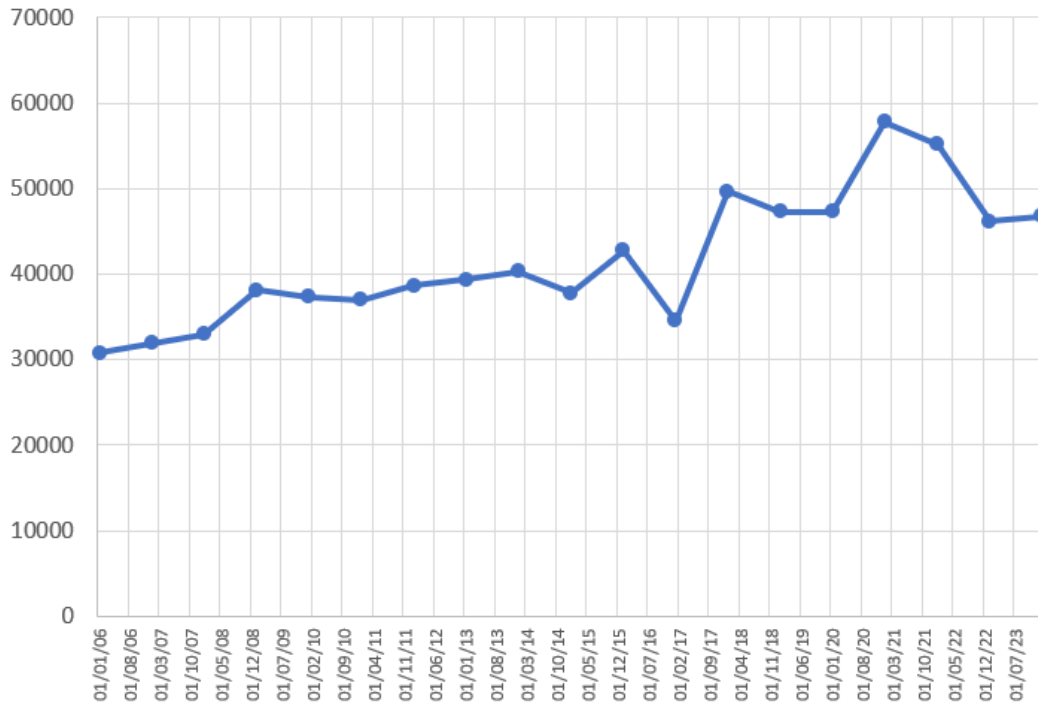
**Cash on Hand 31.12.2023**

**398.25**

### Fluctuation of membership dues



### Capital of the SGK (CHF)



## SGK financial situation 2024

### SGK financial situation 2024

<b>Credits:</b>		<b>Debits:</b>	
Membership dues (until 31/08)	4'420.33	Zürich School of Crystallography	2'000.00
SCNat contribution 2023	10'984.35	SGK annual meeting (+ poster prize)	3'000.00
<b>Total Income</b>	<b>15'404.68</b>	Erice International School	1'500.00
		Workshop on Crystal Growth (PSI)	1'500.00
		Travel grants for students	750.00
		Membership dues to SCNat	1'127.00
		<b>Flack Lecture series (2023)</b>	<b>1'400.23</b>
		Publication costs	127.85
		ECA membership	172.43
		Bank charges	84.08
		Consulting (organization of EPDIC19)	756.70
		Flowers	164.50
		<b>Total Expenses</b>	<b>12'582.79</b>

### SGK financial situation 2024

<b>Expected Credits:</b>		<b>Pending costs :</b>	
Membership dues (until 31/08)	250.00	Travel grants	1'000.00
		Satellite workshop	2'500.00
		Publication costs	750.00
		Bank charges	30.00
		<b>Expected balance at the end of 2024</b>	<b>-1'208</b>

## 3d) Budget for 2025

### SGK Budget proposal 2025

<b>Credits:</b>		<b>Debits:</b>	
Membership dues	5'000.00	Membership dues to SCNat	1'150.00
SCNat - reimbursement ECA delegate	500.00	ECM delegate	1'000.00
SCNat - contribution for SGK annual meeting		SGK Annual meeting + poster prize	3'000.00
	2'500.00	SGK support to PSI School	2'000.00
SCNat - contribution to PSI School	2'000.00	SGK Topical Workshop	3'000.00
SCNat – contribution to Topical Workshop	2'500.00	Travel Grants for Young Scientists	3'500.00
SCNat - PhD / master students travel grants	2'500.00	Howard Flack Lecture Series	4'000.00
SCNat - Crystallographic Lectures:		<b>Preliminary costs of the EPDIC19</b>	<b>5'000.00</b>
Howard - Flack Lecture Series	3'000.00	ECA national membership dues 2023	200.00
SCNat - Publication costs	500.00	Publication costs	1'200.00
Bank interests	100.00	Bank charges	200.00
<b>Total Income</b>	<b>18'600.00</b>	<b>Total Expenses</b>	<b>24'250.00</b>
		<b>Income – Expenses</b>	<b>-5'650.00</b>

### **Membership fees:**

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 2024.

**As per the bylaws, the Assembly is required to vote on the presented financial reports and membership fees.**

**VOTING: The annual financial report 2024, presented by the Treasurer Enrico Giannini, is approved unanimously, without abstentions.**

**VOTING: The Budget forecast 2025, presented by the Treasurer Enrico Giannini, is approved unanimously, without abstentions.**

**VOTING: The prolongation of the current fees for 2025 is approved unanimously, without abstentions.**

### **Elections**

#### **Confirmation of current board members**

- **P. Abdala, N. Casati, E. Giannini, S. Grabowsky, P. Schouwink**
- outgoing member: **D. Sisak-Jung**

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

a) New nominations for the board:

**Céline Besnard** (University of Geneva)

**VOTING: Céline Besnard is accepted as a Board member unanimously, without abstentions.**

b) Change of presidency: proposition Simon Grabowsky (University of Bern)

**VOTING: Simon Grabowsky is accepted as the president unanimously, without abstentions.**

c) Confirmation of auditors:

Antonia Neels, Bernhard Spingler

**VOTING: Bernhard Spingler as Auditor confirmed, and Antonia Neels as Auditor is replacing Kurt Schenk.**

d) Confirmation of delegates to ScNat

- ScNat: S. Grabowsky (automatically assigned to acting president)

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

**5- 2025 Meeting and General Assembly. Decision on location and date: Lausanne, September 10<sup>th</sup> (Dinner Sep 9<sup>th</sup>)**

Minutes written by the Secretary, Paula Abdala, and approved by the President, Simon Grabowsky.

## Highlighted Events

2025 Crystallographic Howard Flack Lecture Series



# Swiss Society for Crystallography

## The Howard Flack Crystallographic Lecture Series

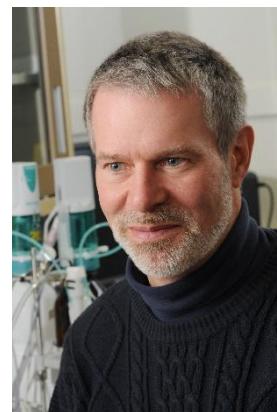
On the topic:  
Mineral Evolution and Mineral Informatics

The 2025 Howard Flack Lecture Series will focus on mineral evolution and the role of minerals in the evolution of life with Professor Robert M. Hazen as our invited Flack Lecturer. Bob uses advanced analytical methods based on crystal structures, compositions, and physical properties to make data-driven discoveries that cover a broad range of disciplines beyond the Earth sciences (theoretical physics, philosophy, linguistics, engineering, soil ecology, cancer research, and more).

**Professor Robert M. Hazen, Carnegie Science  
ETH Zurich (Nov 10), PSI (Nov 11), Bern (Nov 12),  
Uni Lausanne (Nov 13), Geneva (Nov 14)**

Abstracts for both talk topics are on the following page. A more detailed schedule will be published soon on [swiss-crystallography.ch/en/flack\\_lectures](https://swiss-crystallography.ch/en/flack_lectures).

Robert M. Hazen, Staff Scientist at the Earth and Planets Laboratory of Carnegie Science in Washington, DC, and Robinson Professor of Earth Sciences, Emeritus, at George Mason University, received degrees in geology from MIT and Harvard. Author of more than 500 articles and books on science, history, and music, Hazen has been recipient of numerous awards, including the 2021 IMA Medal, the 2016 Roebling Medal of the Mineralogical Society of America, and the 2012 Virginia Outstanding Faculty Award. His book *The Story of Earth* (Viking-Penguin) was finalist in the Royal Society and Phi Beta Kappa science book competitions. The biomineral “hazenite,” as well as a fossil dolphin and a fossil hermit crab, were named in honor of Robert and Margaret Hazen. Since 2008, Hazen and his colleagues have explored “mineral evolution” and “mineral informatics”—new approaches that exploit large and growing mineral data resources to understand the co-evolution of the geosphere and biosphere. In October 2016 Hazen retired from a 40-year career as a professional trumpeter, during which he performed with numerous ensembles including the Metropolitan Opera, Royal Ballet, and National Symphony.

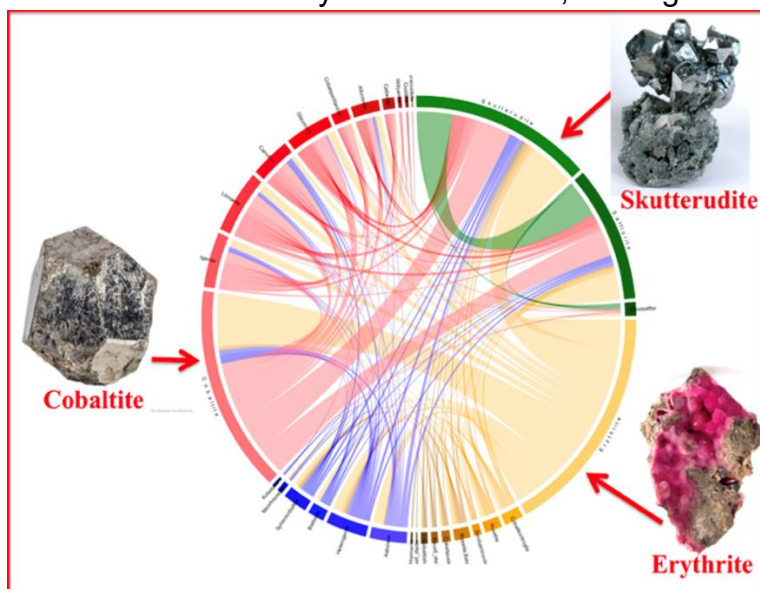


**Robert M. Hazen—Lecture #1**  
**Mineral evolution and the search for critical resources,  
life's origins, and time's second arrow**

Minerals, which display dramatic increases in diversity and complexity through more than 4.5 billion years of Earth's evolution, provide a quintessential example of an abiotic evolving system. Quantitative studies of mineral evolution rely on large and robust mineralogical data resources, including crystal structures, compositions, and physical properties. These data, coupled with advanced analytical and visualization methods, enable us to search for new deposits of critical resources, to probe near-surface environments thought to have influenced the origins of life, and to suggest a framework that unifies behaviors of both biotic and abiotic evolving systems. We posit that all such systems are characterized by combinatorial richness subject to selection—characteristics that hint at a second arrow of time.

**Robert M. Hazen—Lecture #2**  
**Data-Driven Discoveries in Mineralogy**

The story of Earth is a 4.5-billion-year saga of dramatic transformations, driven by physical, chemical, and biological processes. The co-evolution of life and rocks unfolded in an irreversible sequence of evolutionary stages. Each stage re-sculpted our planet's surface, while introducing new planetary processes and phenomena. This grand and intertwined tale of Earth's living and non-living spheres is coming into ever-sharper focus, thanks to advances in “mineral informatics”—a field that employs large and growing mineral data resources to tell the deep-time stories of our evolving planet. Minerals are remarkably information rich, holding dozens of trace and minor elements,



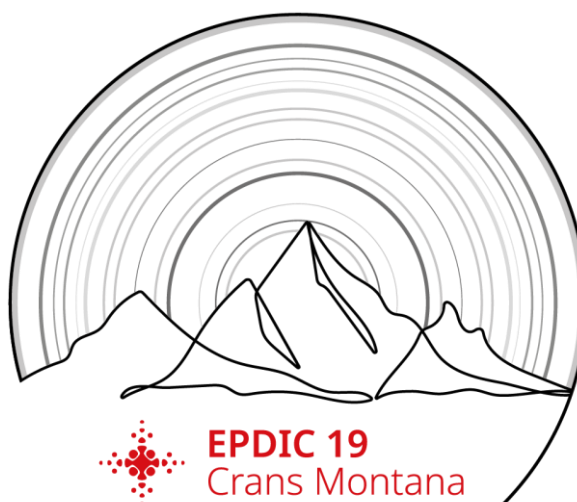
scores of stable isotopes, solid and fluid inclusions, chemical zoning, twinning, exsolution, countless defects, and a host of optical, magnetic, electrical, and other properties. Every mineral specimen is a time capsule waiting to be opened—waiting to tell its story. This lecture will explore some of the advanced data analytical and visualization methods that are shining new

light on the old field of mineralogy.

**CRANS MONTANA | 23-26 JUNE 2026**

Welcome to EPDiC19, welcome to Crans Montana!

On Behalf of the Permanent International Committee of EPDiC, EPDiCCom, it is our pleasure to invite you to join us for the 19th European Powder Diffraction Conference, which will take place in the heart of the Swiss Alps from June 23<sup>rd</sup> – 26<sup>th</sup>, in Crans Montana.



EPDiC is a cornerstone in the field of powder diffraction, and has long served as a vital platform for the exchange of scientific knowledge on the broader topics spanning materials science and the advances of experimental techniques. The promotion of cross-disciplinary and inter-generational exchange is at the heart of EPDiC, as is fostering the participation of young scientists. EPDiC brings together leading experts, early career researchers as well as industry professionals, and contributes significantly to strengthening the global community in this field.

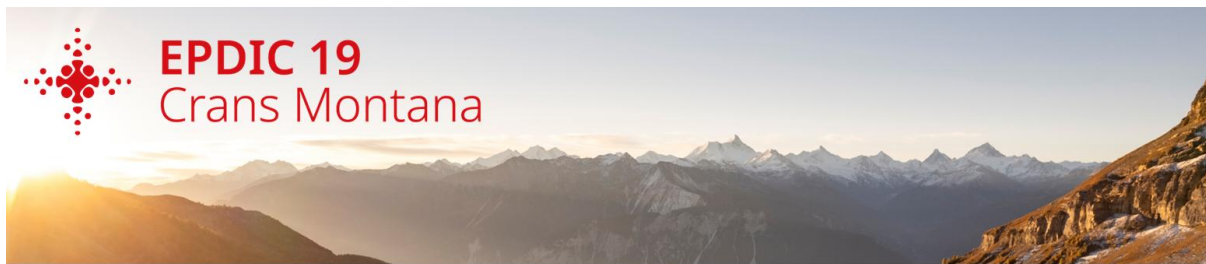
Crans Montana is a beautiful destination embedded in the mountains of the Valais, close to the borders of Italy and France, as well as to the Lake of Geneva region, and surrounded by breath-taking panoramic views. Crans Montana will provide the perfect setting for an exciting scientific program, fruitful exchange and casual get-together during the days of EPDiC19, and promises you an unforgettable stay.

Pascal Schouwink,  
Chair  
Antonia Neels, Radovan Cerny  
and Co-chairs of EPDiC19

Jasminka Popović  
Chair of the EPDiC Committee



# EPDIC 19 Crans Montana



## 19<sup>th</sup> European Powder Diffraction Conference

The 19<sup>th</sup> European Powder Diffraction Conference (EPDIC19) will take place in the heart of the Swiss Alps, Crans Montana, from 23 to 26 June 2026.



### Microsymposia

### Organized by

EPDIC Committee and the Swiss Society for Crystallography (SSCr)

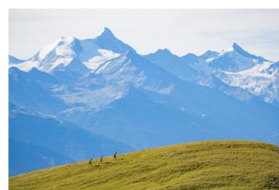
Pascal Schouwink (Chair), Antonia Neels (co-Chair), Radovan Cerny (co-Chair)

Chair of the EPDIC Committee:  
Jasminka Popovic

### Venue

Conference Center Le Régent  
[www.crans-montana.ch/congres](http://www.crans-montana.ch/congres)

- The current state and prospects of functional materials
  - In situ and operando studies
- Structure and dynamics in disordered materials
- Materials for energy conversion and storage
- Innovation in structure solution and refinement
  - Nanomaterials, surfaces, and interfaces
  - Pharmaceutical and biological materials
  - Magnetic structures and neutron scattering
- Combining complementary techniques for structural Studies
  - Microstructure, texture, and line profile analysis
  - Artificial Intelligence for powder diffraction
- Quantitative analysis: state of the art and new perspective



[www.epdic19.com](http://www.epdic19.com)  
[info@epdic19.com](mailto:info@epdic19.com)



Swisscrystallog



SSCr-Swiss Society for Crystallography



## Calendar of Events



### **PSI Synchrotron Powder Diffraction School**

15-19 September, 2025



PSI, Villigen



<https://www.epfl.ch/research/domains/ccmx/courses-and-events/2025pds/>



### **The Zurich School of Crystallography 2026: Bring Your Own Crystals**

17-27 Jun 2026



University of Zurich, Switzerland



<https://www.chem.uzh.ch/linden/zsc/>



### **IUCr 2026 Congress**

11-18 August 2026



Calgary, Canada;



<https://www.iucr2026.org/>



### **The European Powder Diffraction Conference EPDIC19**

23-26 June 2026



Crans Montana



Tba/ <https://swiss-crystallography.ch/en>

## 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
<b>SLS-2</b>		
Debye, ADDAMS, PoILux, SuperXAS, PXII	20.08.2025	
Mesquik	Contact BL scientist	
<b>SINQ/SLS-2</b>		
Joint x+n proposals (MS/HRPT)	Suspended	
<b>SINQ</b>		
All instruments regular calls	15.05, 15.11	<a href="https://www.psi.ch/de/useroffice/proposal-deadlines">https://www.psi.ch/de/useroffice/proposal-deadlines</a>
<b>SμS: Swiss Muon Source</b>		
FLAME, GPD, GPS, HAL-9500, LEM	02.06	
DOLLY, FLAME, GPD, GPS, HAL-9500, LEM	01.12	
<b>SwissFEL</b>		
ARAMIS-Alvra, ARAMIS-Bernina	15.03, 15.09	
<b>ESRF</b>		
Standard, BAG proposals	01.03, 10.09 (17h) Note new template	<a href="https://www.esrf.fr/home/UsersAndScience/Apply-for-beamtime/proposal-types-and-deadlines.html">https://www.esrf.fr/home/UsersAndScience/Apply-for-beamtime/proposal-types-and-deadlines.html</a>
Long Term Project, HUB proposals	15.01 (17h)	
CRG SNBL	01.03, 10.09 Access via CRG mode (only Swiss and Norwegian groups can apply)	<a href="http://www.esrf.fr/UsersAndScience/Experiments/CRG/BM01#">www.esrf.fr/UsersAndScience/Experiments/CRG/BM01#</a> Contact: wouter@esrf.fr
<b>ILL</b>	17.2, 15.9	<a href="http://www.ill.eu/users">www.ill.eu/users</a>
<b>FRM II</b>	tba	<a href="http://www.mlz-garching.de/user-office/">http://www.mlz-garching.de/user-office/</a>
All instruments/ Rapid access program		
<b>DESY</b>	01.03, 01.09 plus rolling access	<a href="https://photon-science.desy.de/users_area/calls_deadlines/index_eng.html">https://photon-science.desy.de/users_area/calls_deadlines/index_eng.html</a>

## Travel Grants for SSCr Members

**Our Society supports members participating in 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 are PhD and Master students. They can receive 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 programme does not permit participant presentations, can be supported with up to CHF 500.

Postdocs can be supported only for oral presentations with a maximum of CHF 500. Per institute and year, a maximum of two people can be supported. There are no strict submission deadlines for travel grant applications, requests will be reviewed upon submission. We advise you to submit as early as possible in the year.

Please submit applications to the President of the Society at [swiss-crystallography@gmail.com](mailto:swiss-crystallography@gmail.com) including the following documents:

- Conference abstract if applicable
- Type of presentation/involvement (poster, talk or workshop/school without presentation)
- Letter of motivation (specify the date you first joined the SSCr)
- Letter of support from your supervisor
- Brief budget of expected costs of attending the meeting

**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, but not exceeding CHF 750.

Please submit applications to the President of the Society at [swiss-crystallography@gmail.com](mailto:swiss-crystallography@gmail.com) including the following documents:

- Conference abstract if applicable
- Type of presentation/involvement (presentation, lecture, session chair, organizer)
- Brief budget of expected costs of attending the meeting

The board of the SSCr wishes you an exciting year with lots of scientific exchanges around the world!

## Institutional members and supporting institutions

### Corporate members

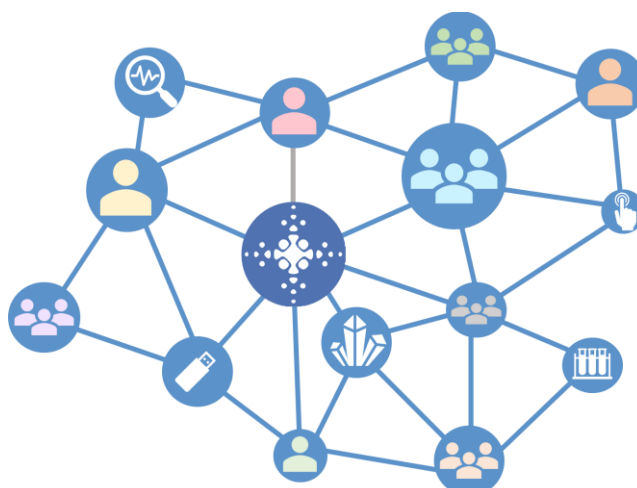


### Supporting institutions



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

## Become a member of the SSCr!





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

For more information as well as online registration, please go to our website <https://swiss-crystallography.ch/en/membership>

The yearly membership fee is CHF 40 for regular members and CHF 10 for students. SGK/SSCr is a member of the Swiss Academy of Science.

### Connect with us!

Web: <https://swiss-crystallography.ch/en>  
E-mail: [swiss.crystallography@gmail.com](mailto:swiss.crystallography@gmail.com)  
 [Swisscrystallog](#)  
 [SSCr-Swiss Society for Crystallography](#)

## Members of the Board of the SSCr for the period 2024 – 2025



Céline Besnard  
**Web Manager**  
University of Geneva



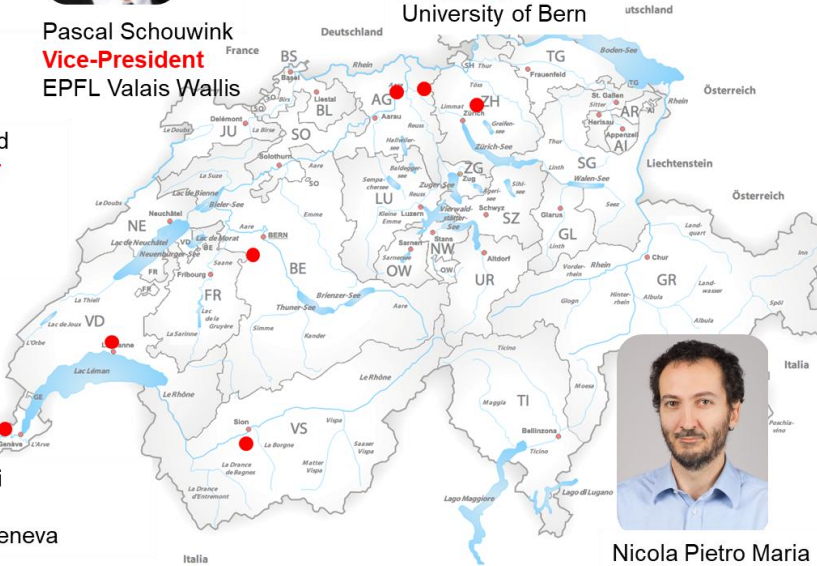
Pascal Schouwink  
**Vice-President**  
EPFL Valais Wallis



Simon Grabowsky  
**President**  
University of Bern



Enrico Giannini  
**Treasurer**  
University of Geneva



Paula Abdala  
**Secretary**  
LESE-ETHZ



Nicola Pietro Maria Casati  
**Events organization**  
Material Science Group PSI

### Candidate for the next period:



Dr. Ekaterina Pomjakushina  
CNM, PSI

### Auditors:



Prof. Dr. Bernhard Spingler  
University of Zurich



Prof. Dr. Antonia Neels (EMPA)

## Contact details of the SSCr Board Members

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SGK/SSCr Newsletter (ISSN 1662-5358, online version: ISSN 1662-534X)

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BIC: UBSWCHZH80A

BLZ: 279

Printing and

Mailing:



Eidgenössische Technische Hochschule Zürich  
Swiss Federal Institute of Technology Zurich

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The newsletter of SGK/SSCr is published 2-3 times a year with a circulation of 250. Contributions are welcome at any time, as well as illustrations for the cover. Articles in English, German or French may be submitted. Please send all interesting material directly to the editor.

Commercial advertisements of material of interest to members of the SGK/SSCr are welcome. Please contact the treasurer for details of the advertising rates.