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Dear Readers

We would like to begin this preface with a few words in memory of Professor Wojciech Paszkowicz, who passed away in October 2025. Professor Paszkowicz was an outstanding crystallographer, materials scientist, and a highly respected member of the Polish synchrotron community. For many years affiliated with the Institute of Physics of the Polish Academy of Sciences, he made important contributions to the structural characterization of materials using laboratory and synchrotron-based diffraction techniques, particularly in semiconductor physics, crystallography, and materials science. His scientific interests encompassed structural studies of functional materials, lattice properties, phase transitions, and advanced approaches to crystallographic analysis. He authored and co-authored nearly 400 scientific publications, leaving a lasting impact on several areas of condensed matter and materials research. Professor Paszkowicz was not only an outstanding scientist but also a very dedicated member of the Polish synchrotron community. He was the founding editor and long-standing Editor-in-Chief of Synchrotron Radiation in Natural Science, creating an important forum for disseminating scientific achievements related to synchrotron and free-electron laser research in Poland. He was also actively involved in scientific committees and initiatives supporting synchrotron science and international cooperation. Beyond his scientific accomplishments, Professor Paszkowicz will be remembered as a thoughtful colleague and mentor.

The present volume is published at a moment of both reflection and progress for the Polish synchrotron community. While remembering those who helped shape its foundations, we also witness a period of development of large-scale research infrastructures and increasing international visibility of Polish synchrotron and free-electron laser science.

In 2025, SOLARIS further consolidated its role as Poland’s flagship synchrotron facility and an increasingly important partner within the European framework of photon, neutron, and free-electron laser infrastructures. The expansion of beamline capabilities, commissioning of new experimental stations such as CIRI, progress on strategic projects including ARYA, MAVKA, and SMAUG, all demonstrate the operational maturity and scientific ambition of the Centre. Beyond infrastructure, SOLARIS has become an active architect of European research policy through its leadership within the LEAPS Consortium and its visible engagement in shaping future European research infrastructure strategies.

A particularly important aspect in this volume is SOLARIS's coordination of the NEPHEWS Project. NEPHEWS represents one of the most ambitious Horizon Europe initiatives dedicated to integrating access to neutron, synchrotron, and free-electron laser facilities across Europe. By connecting 20 major research infrastructures, user organizations, and more than 40,000 researchers, the project strengthens transnational access and supports early-stage researchers. SOLARIS, as the coordinator of this initiative, facilitates access to world-leading facilities but also actively shapes the future of European scientific collaboration, grounded in openness, mobility, and excellence.

The 10^{th} anniversary of the SOLARIS National Synchrotron Radiation Center's operations was celebrated on 22nd May. The anniversary provided an opportunity to summarize a decade of dynamic development, including the commissioning of new beamlines, the expansion of international collaborations, and a continuous increase in the number of users representing diverse scientific disciplines.

The long-standing and fruitful collaboration with the European Synchrotron Radiation Facility (ESRF) remains important, as it is one of the most significant international partners for Polish scientists. This volume presents some examples of research enabled by ESRF access—from high-pressure crystallography and charge-density studies of hydrogen-bond symmetrization in natrochalcite, to investigations of amorphous pharmaceuticals and operando studies of electrochemical graphene oxide synthesis. The institutional dialogue between ESRF and the Polish scientific community, strengthened through recent high-level visits, further confirms the strategic importance of this partnership.

The issue also emphasizes the growing relevance of free-electron laser science in the broader European research landscape, particularly through collaboration with facilities such as the European XFEL. It is our pleasure to announce that Prof. Ryszard Sobierajski (Institute of Physics of the Polish Academy of Sciences) was elected as the next Chair of the XFEL Council, effective 1st July 2026, an important event for the Polish scientific community involved in large-scale research infrastructures.

The articles collected in this volume illustrate the large synchrotron research, from structural chemistry and condensed matter physics to materials science, catalysis, life sciences, and green energy technologies.

On behalf of the Editorial Board, we thank all authors, reviewers, and contributors for their valuable work and dedication in preparing this issue. We invite you to explore Volume 26 of Synchrotron Radiation in Natural Science.

Edyta Piskorska-Hommel

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SOLARIS in 2025: Infrastructure Development and European Collaboration

Agnieszka Cudek[1], Adriana Wawrzyniak[1], Michał Młynarczyk[1], Marcin Sikora[1]

[1]SOLARIS National Synchrotron Radiation Centre

In Stanisław Lem's novel *Solaris*, an encounter with the unknown begins with careful observation—an attempt to understand phenomena that resist simple description. In the world of science and technology, 2025 was likewise a year of acceleration, change, and the redefinition of priorities: in Europe and globally, the need for technological sovereignty, resilient systems, and investment in solutions capable of addressing energy, health, and geopolitical challenges became increasingly pronounced. Against this backdrop, the SOLARIS National Synchrotron Radiation Centre consistently expanded its infrastructure and strengthened its position within Europe's ecosystem of large-scale research infrastructures, becoming an ever more active participant in joint initiatives and projects. The past year brought not only further stages of the Centre's development and growing user activity, but also an intensification of international cooperation.

Infrastructure development and beam availability

For the Accelerators Division, 2025 was a period of intensive operational work and dynamic technological development, with the overarching goal of providing a stable, reliable, high-quality photon beam for beamline users. The Division successfully delivered on its core mission while simultaneously expanding accelerator infrastructure, diagnostic capabilities, and engineering and R&D capacity.

A key organizational step was extending user beamtime to six days per week by adding Sundays to the operational schedule. As a result, experiments at SOLARIS could be carried out over a larger part of the week, while still retaining one day dedicated to optimization and upgrade work. The storage ring was routinely refilled twice per day, and the planned winter and summer shutdowns enabled the necessary inspections and upgrades of accelerator systems. Despite the increased operational load, beam availability remained high in 2025 at 96.8%. The mean time between failures (MTBF) was 76.3 hours, while the mean time to repair (MTTR) was only 1.7 hours. Slightly lower indicators compared to the previous year were primarily related to failures of the main RF power supply units of the linear accelerator and intermittent issues with the synchrotron cooling system.

The Accelerators Division carried out a broad range of operational and diagnostic activities, including tests of different accelerator operating modes, advanced beam measurements, and the development of diagnostic tools. Analyses and simulations required for new insertion devices were performed, diagnostic systems were calibrated, and work progressed on the ARYA and MAVKA beamline projects as well as the POLFEL accelerator. In parallel, operational and diagnostic software in the Python environment was developed, measurements were conducted for the future tune feedback system, and advanced signal analyses from beam loss monitors were initiated.

The most significant engineering achievement of the year was the completion of a 100 MHz pulsed amplifier (chopper) for the linear accelerator, designed and built entirely by the SOLARIS team. Delivered with 100% in-house contribution, the project represented a major technological challenge and confirmed the team's high competence in designing advanced RF systems, diagnostics, interlocks, and ergonomic user interfaces.

In 2025, substantial progress was also made in orbit stabilization systems, in particular the FOFB Watchdog programme, as well as in the area of imaging detectors for the Lumos beamline and the future Pinhole beamline. The developed solutions feature high dynamic range, flexible configuration, and full integration with the TANGO control system, providing a solid basis for further development of diagnostic infrastructure. A significant part of the Division's activities consisted of service and infrastructure work, including modernization of LLRF systems, modulator repairs, klystron replacements, work on the ARYA and CIRI beamlines, and the replacement of the HAB absorber on the POLYX beamline. In parallel, efforts continued to expand measurement and metrology capabilities. In 2025, dedicated measurement setups for characterizing magnets and insertion devices were constructed, significantly increasing the Centre's autonomy in precision magnetic measurements. The delivery and testing of a three-pole wiggler for the SOLCRYS beamline were also completed, confirming its parameters and readiness for further integration with accelerator infrastructure. An integral component of these activities was advanced modelling and analysis of insertion devices using the finite element method (FEM), enabling optimization of their design and assessment of their impact on beam parameters. Additional work included miniaturization of the system for measuring magnet curvature, enhancing diagnostic capabilities while reducing the size and complexity of the apparatus. In parallel, construction began on a magnetic laboratory, which in the coming years will become a key element of the research and development infrastructure.

Complementing the technical work was the strong presence of Accelerators Division staff at international conferences and workshops, where results were presented, experience was shared, and teams actively participated in international knowledge exchange. A further outcome of these efforts includes publications in conference proceedings (IPAC25 Proceedings and IBIC'25 Proceedings).

In summary, 2025 confirmed the operational maturity and high competence of the Accelerators Division. It was a year of successfully combining reliable user operations with ambitious technological and R&D development, providing a solid foundation for the continued growth of the SOLARIS National Synchrotron Radiation Centre in the years to come.

Users and research publications

The past year was a time of further intensive development for the SOLARIS National Synchrotron Radiation Centre and of strengthening its position on the European scientific landscape. Once again, the number of access cards issued to external users for the duration of their experiments exceeded 1,000. With the extension of synchrotron user operation to six days per week, users can apply for beamtime for a single experiment of up to 144 hours, which is a standard at leading facilities of this kind worldwide.

To broaden awareness of the synchrotron's research capabilities, researchers from the Scientific Division participated in SOLARIS open days at the Warsaw University of Technology and at the Faculty of Chemistry of the Jagiellonian University. Similar events are planned for 2026 in Toruń, Gdańsk, and Wrocław. In addition, a pilot programme was introduced to reimburse travel costs for early-career researchers conducting experiments at SOLARIS. This is a form of support that we hope to extend to a wider group of users in the near future.

One of the most significant milestones in research infrastructure development was the official commissioning of the CIRI beamline, whose three experimental stations enable chemical imaging of materials at micro- and nanometer scales using synchrotron radiation in the infrared range. The expanded experimental hall also saw the arrival of the first components of the SMAUG beamline, dedicated to research using small-angle scattering of hard X-rays. Notably, this beamline is already accepting proposals for test experiments.

In the new part of the hall, the first stage of sample preparation laboratories was completed; these will soon be made available to users conducting advanced experiments in biology, biochemistry, chemistry, and surface physics. Construction of the helium recovery installation was also completed, and installation of the helium liquefier is expected to be finished at the beginning of the following year. This investment will significantly expand the Centre's capabilities for research on quantum and magnetic materials.

Also in the new part of the hall, work is advancing on the MAVKA synchrotron beamline, being built through cooperation among European synchrotrons within the LEAPS consortium as part of efforts to support the development of the Ukrainian synchrotron community. The first elements of this beamline are expected to reach SOLARIS from the Swiss Light Source (SLS) in 2026. The ARYA beamline, dedicated to protein crystallography, is also at an advanced stage of construction—its first components, including the wiggler, have already been delivered. We hope that once ARYA is opened, SOLARIS will host a unique infrastructure environment for structural biology, comprising the SMAUG and ARYA beamlines and cryo-electron microscopy, which was upgraded through the purchase of a latest-generation direct electron detection camera with an energy filter.

Alongside continuous infrastructure development, 2025 also saw a growing body of scientific publications produced by users of the SOLARIS infrastructure. Many papers appeared in journals with very high impact and visibility. These include publications in *Nature Communications*, *Nature Microbiology*, *Journal of the American Chemical Society*, *ACS Nano*, *Small*, *Acta Materialia*, and *Chemistry of Materials*. A complete, continuously updated list of scientific articles is available on the SOLARIS website in the "Research" section. Among the results published in 2025, it is worth noting the particularly large number of studies on materials for green energy—covering new generations of batteries, catalysts, and cells. Of growing interest are studies on hydrogen technologies using solid oxide fuel cells. A team of scientists from the Faculty of Applied Physics and Mathematics of the Gdańsk University of Technology, in collaboration with researchers from the PIRX and ASTRA beamlines, investigated ways to increase the stability—and thus extend the lifetime—of this type of cell through lanthanum doping. The results were published in *Nanoscale*.

Unique results also emerged from the first months of research on the recently opened POLYX beamline. A team from AGH University of Science and Technology, the Jagiellonian University, and the R&D department of INGLOT developed a method using synchrotron light to detect lead in intermediates used in cosmetics production. The results were published in the specialist journal *Spectrochimica Acta Part B: Atomic Spectroscopy*. We hope that cooperation with the synchrotron will help maintain high standards of chemical safety for cosmetics produced by Polish manufacturers.

Events, international cooperation, and strategic projects

In 2025, the Centre continued its intensive activity in the areas of international cooperation, strategic dialogue at the European Union level, and support for processes shaping science policy and research infrastructure development. These efforts aligned with the broader context of the European Research Area and ongoing discussions on the future funding of research and innovation under the 10th Framework Programme (2028–2034).

SOLARIS actively participated in initiatives related to dialogue with European institutions, including consultations and meetings devoted to mechanisms for supporting research infrastructures and long-term directions for their development. A particular focus for the Centre remains the policy of open access to pan-European research infrastructures and ensuring equal opportunities for scientists regardless of their location. In parallel, the Centre supported national authorities in preparing and articulating Poland's positions on research infrastructure development strategies, emphasizing the role of large, unique facilities as the foundation of a modern research and innovation system. An important element of these activities was also mobilizing the national community—universities, institutes, and other stakeholders in the science system—in the debate on the future EU budget for research and development, including participation in developing the position of the Main Council of Science and Higher Education.

At the same time, 2025 continued a strong track record in the implementation of international projects. SOLARIS successfully advanced the RIANA project in nanotechnology, strengthening access to advanced research infrastructures, and continued work on the flagship NEPHEWS project, coordinated by the SOLARIS Centre. This project remains one of the key undertakings integrating European competences in synchrotron-based research.

New European project initiatives also joined the SOLARIS portfolio. The RIFF project—*Research Infrastructures for the Future of Ukraine: Roadmap for Sustained Growth and Recovery*—focuses on consolidating European research infrastructures to support research infrastructure development policy in Ukraine, contributing to efforts to rebuild and strengthen the Ukrainian research system. The GREEN-MEM project—*Green materials for sustainable* *magneto-electronic memories*—is aimed at developing a new generation of magneto-electronic memory materials based on non-critical, environmentally friendly raw materials with high availability and diversified geographical origin. The past year also saw the completion of the LEAPS-INNOV project, integrating European synchrotron and free-electron laser infrastructures around key scientific and technological challenges, complemented by a strong component of cooperation with industry. SOLARIS's participation in this undertaking strengthened the Centre's competences in knowledge and technology transfer and in cooperation with the economic environment.

In parallel, SOLARIS developed solidarity-driven international cooperation in response to geopolitical challenges. The Centre joined the international coalition for Ukraine initiated by the European Commission, engaging in activities aimed at supporting Ukrainian scientists and further integrating them into the European research system.

In 2025, the Centre also clearly marked its presence on the map of European scientific and infrastructure cooperation, becoming a host and active participant in events of strategic importance to the entire research community. One of the key highlights of the year was three days of intensive meetings in Kraków within the framework of the 3rd ESFRI Stakeholders Forum Meetup and the 92nd ESFRI Forum Plenary Meeting, organized in close cooperation with ESFRI and the Ministry of Science and Higher Education. Discussions addressed, among other topics, the long-term sustainability of Europe's research infrastructure ecosystem, synergies in funding, and the role of RI–industry cooperation. The event was included in the official calendar of Poland's Presidency of the Council of the European Union, underscoring the growing importance of Poland and the region in shaping European research and innovation policy. At the same time, SOLARIS hosted important European partners, including workshops by the European Science Foundation and the Europlanet Society devoted to the role of small and medium-sized infrastructures in maintaining Europe's research competitiveness, as well as events under the RICH Europe project, aimed at professionalizing and harmonizing National Contact Point activities and strengthening cooperation between ESFRI structures and international partners. In June, SOLARIS also hosted strategic LEAPS meetings—the RDB, General Assembly, and Task Force—focused on planning the consortium's further development and work on the "LEAPS Technology Road Map", defining technological priorities for European light sources.

A significant space for building international relationships and connecting science with industry was the LEAPS Meets Advanced Materials for Energy 2025 conference, organized by SOLARIS in Sopot. The event gathered around 80 participants and focused on the use of synchrotron radiation in research on energy materials, highlighting the importance of interdisciplinary cooperation for the development of sustainable energy technologies.

For the SOLARIS National Synchrotron Radiation Centre, 2025 was a year of exceptionally strong engagement and genuine responsibility for the direction of the LEAPS consortium. The Director of SOLARIS served as Chair of the Board, actively steering the consortium's work and co-shaping its strategic priorities in the development of European light sources. During this period, SOLARIS acted as host and initiator of many key LEAPS meetings and also led selected working groups, supporting coordination in the most important areas of cooperation. The Centre's activity was also visible on the international stage at the RTI Summit 2025 in Copenhagen, where SOLARIS promoted LEAPS as an important partner in the European Research and Technology Infrastructures ecosystem, emphasizing the importance of joint investments and shared resources for Europe's competitiveness. An additional strengthening of SOLARIS's role within the consortium structure was the assumption of coordination of LEAPS communications, enabling even more effective enhancement of the visibility and impact of joint activities across Europe.

Undoubtedly, the actions undertaken in the past year contributed to further strengthening the scientific and institutional potential of the SOLARIS Centre, increasing its capacity to effectively implement projects financed by national and European funds and to actively participate in shaping good practices and cooperation in the field of research infrastructure on the international stage.

Science outreach and public engagement

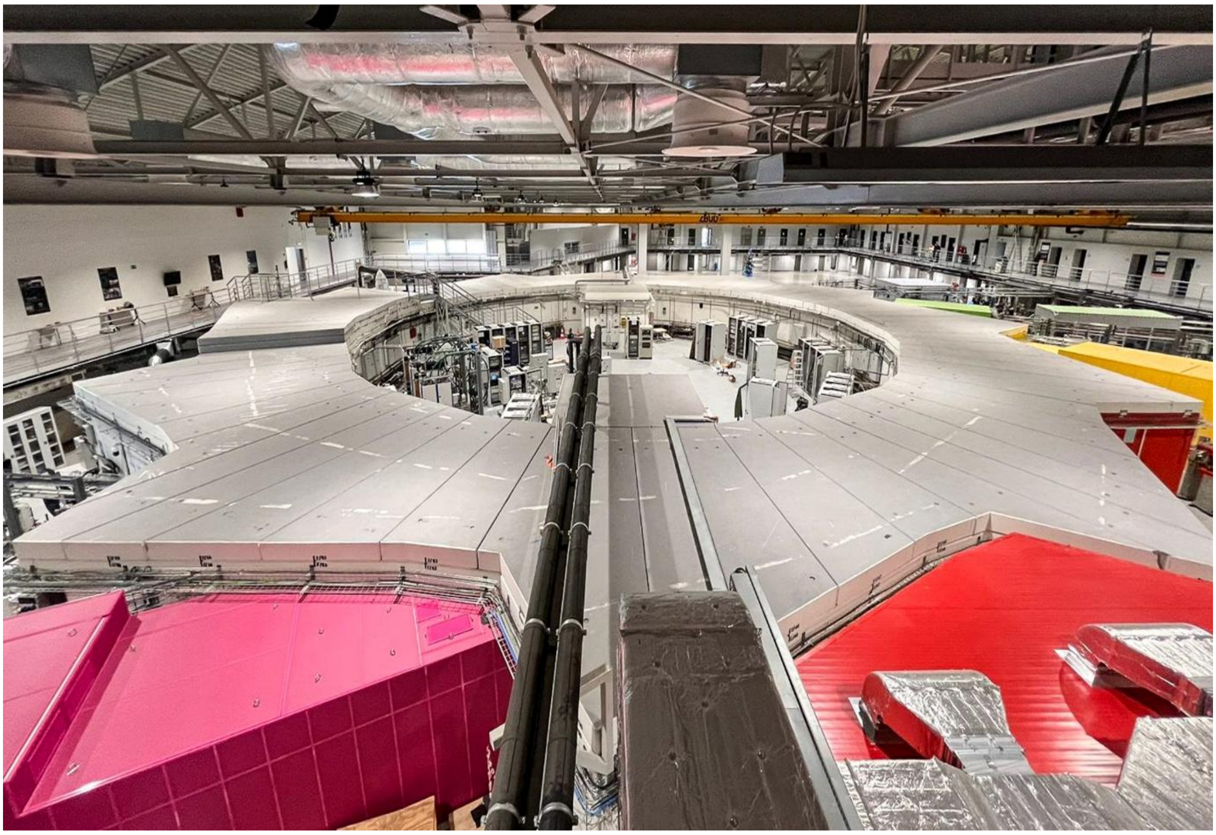
In 2025, the SOLARIS Centre consistently expanded outreach and educational activities, strengthening its presence in public awareness as a place where a modern research infrastructure becomes accessible and understandable also to those outside the scientific community. A key element of this approach was initiatives opening the Centre to a broad audience and presenting science as a direct experience. During the Małopolska Researchers' Night, SOLARIS once again invited participants into the world of synchrotron light, offering, among other activities, lectures, educational games, film screenings, interactive stations, and tours of the infrastructure.

A particularly important pillar of science outreach was the first year of implementing the "Skilla Academy" project, funded by the Ministry of Science and Higher Education under the "Social Responsibility of Science II" programme. The project was designed as a comprehensive programme introducing young people and teachers to the specific nature of a large-scale research infrastructure. As part of educational visits, the Centre welcomed 2,219 participants, who had the opportunity to tour the facility and learn about the work of synchrotron scientists and specialists. The Academy programme also developed a workshop component based on a Game-Based Learning approach. Workshops began in October, and in the first stage 3 of the 30 planned sessions were delivered, with very high interest from schools, clearly exceeding the project's initial assumptions. In parallel, a competition component was launched, including a nationwide contest for students for the best scientific poster illustrating how the synchrotron accelerator system works; the prize for the 30 best classes was free workshops at SOLARIS. A major achievement in educational tools was the completion of work on the original board game "SOLARIS: Scientific Mission", which became a key teaching element of the project. The game presents, in an engaging way, the mechanisms of conducting research on synchrotron beamlines.

Building on this foundation, outreach activities were supported by consistently developed communication through the Centre's own channels and by presence in external media. In 2025, the Centre appeared in national and sectoral media, with over 50 mentions across press, radio, and online services. At the same time, social media activity continued to grow—the total number of followers across Facebook, Instagram, YouTube, X, and LinkedIn reached 6,865, representing a 24% increase compared to the previous year, with LinkedIn once again showing the highest growth rate (+59%). As a result, SOLARIS maintained steady contact with audiences, supporting the visibility of its activities, research, and projects, while strengthening its position as a modern research infrastructure open to dialogue with science, education, and society.

Finally, it is worth emphasizing that 2025 was also a period of systematic development of SOLARIS's institutional competences in public procurement—crucial for the efficient operation of large research infrastructures and the implementation of complex technological investments. Representatives of the Public Procurement Section participated in an international group of specialists bringing together institutions within the LEAPS consortium, co-creating a space for exchanging experience and good practices in conducting procurement procedures.

The Centre also took an active part in conferences and workshops on this topic, presenting papers and further developing team competences, and in the second half of the year began participation in the EU project INPROCAP, comprising a series of trainings aimed at further professionalizing processes. These activities strengthen SOLARIS's ability to effectively deliver national and European projects and to build a stable organizational foundation for the continued development of the infrastructure.



Joanna Kowalik

The NEPHEWS Project – Strengthening Access to European Photon, Neutron, and FEL Facilities

Piotr Piwowarczyk[1], Krzysztof Zieliński[1], Magdalena Żychowska[1]

[1]*SOLARIS National Synchrotron Radiation Centre*

Keywords: user-oriented programmes, curiosity-driven collaboration, neutron and photon facilities, user community building

NEPHEWS - *NEutrons and PHotons Elevating Worldwide Science* is a project funded by the European Commission under the Horizon Europe programme. Is a collaborative initiative aimed at integrating and strengthening the European landscape of photon and neutron research infrastructures (RIs). It is implemented in partnership with 20 RI facilities, united in two largest and most advanced consortia LEAPS (League of European Accelerator-based Photon Sources) and LENS (League of Advanced European Neutron Sources), as well as two user organizations ESUO (European Synchrotron and Free Electron Laser User Organisation) and ENSA (European Neutron Scattering Association), with the National Synchrotron Radiation Centre SOLARIS at Jagiellonian University acting as a coordinator (*Table 1*).

Table 1 – Composition of the NEPHEWS project consortium

<table>
<tr><th colspan="6">Partners of the NEPHEWS project</th></tr>
<tr><td>SOLARIS</td><td>MAX IV</td><td>HZB</td><td>ELETTRA</td><td>DESY</td></tr>
<tr><td>ISA</td><td>ALBA</td><td>MLZ</td><td>UJF</td><td>SOLEIL</td></tr>
<tr><td>HFML FELIX</td><td>TARLA</td><td>HZDR</td><td>ISIS</td><td>PSI</td></tr>
<tr><td>ILL</td><td>EU XFEL</td><td>ENSA</td><td>TCD</td><td>HUN REN EK</td></tr>
<tr><td colspan="2">ESRF</td><td>ESUO</td><td colspan="2">SESAME</td></tr>
</table>

The NEPHEWS project provides access to Europe's leading neutron, synchrotron, and free-electron laser RIs to support scientific excellence. Furthermore, by bringing together facilities, User organisations, and scientific communities representing more than 40,000 Users across Europe, it creates a strong foundation for coordinated access and training activities.

Its main objectives focus not only on expanding access to advanced RIs in general, but also on supporting users from 8 selected countries (Estonia, Finland, Greece, Poland, Portugal, Romania, Serbia and Ukraine), as well as from widening and underrepresented countries and those without direct access to RIs. The project also aims to enhance knowledge transfer between experienced and new Users, strengthen European cooperation between RIs and user organisations, and promote scientific excellence through transnational collaboration and training.

These objectives are achieved through three User-oriented programmes that support researchers at different career stages:

Transnational Access (TNA)

Free-of-charge access to facilities is provided by 14 partner RIs and includes beamtime and technical support. The programme supports both on-site and remgroups andents, enabling broad participation from eligible research groups, and is primarily dedicated to experienced Users who are well advanced with performing experiments at RIs. Although this programme is open to all eligible User groups, project gives priority to researchers affiliated in 8 selected countries, as well as widening, non-facility and underrepresented countries.

Within the NEPHEWS project, researchers not only benefit from free access to RIs which is typical for academia Users but also receive support in the form of reimbursement for travel and accommodation costs.

The project aims to support 902 users under the TNA programme. As of March 2026, it has already achieved strong progress, with 507 users supported, including 183 affiliated with target countries (*Fig. 1*).

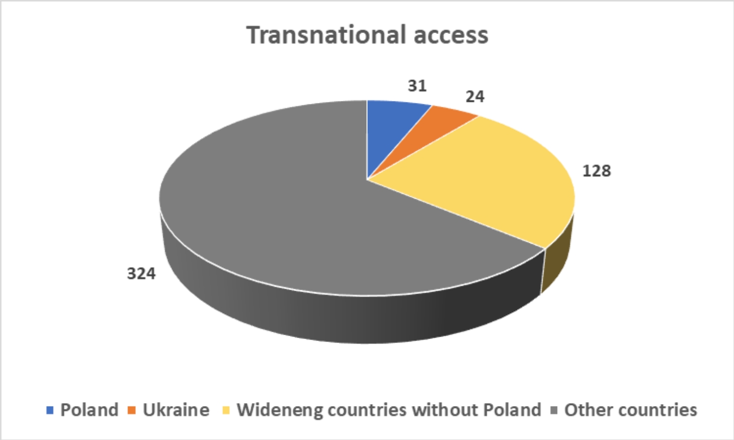


Figure 1. Number of users supported under the TNA programme by country of affiliation

User Twinning Programme

The Twinning Programme is dedicated to new and inexperienced Users who wish to gain knowledge about research techniques and opportunities offered by RIs. Its main objective is to enhance knowledge transfer between a new User and an experienced research group that voluntarily hosts the "novice" during their experiments. This approach guarantees that new Users can gain tailored, first-hand experience.

The NEPHEWS project supports scientists at all stages of their careers. Participants in this programme receive reimbursement for travel and accommodation expenses related to their visits.

Within the NEPHEWS project, the programme is implemented by 18 partner RIs, which will carry out 135 twinning actions. As of March 2026, the number of registered users has reached 134, including 19 participants from Poland (*Fig. 2*).

This programme plays a key role in building long-term user expertise and fostering international collaboration.

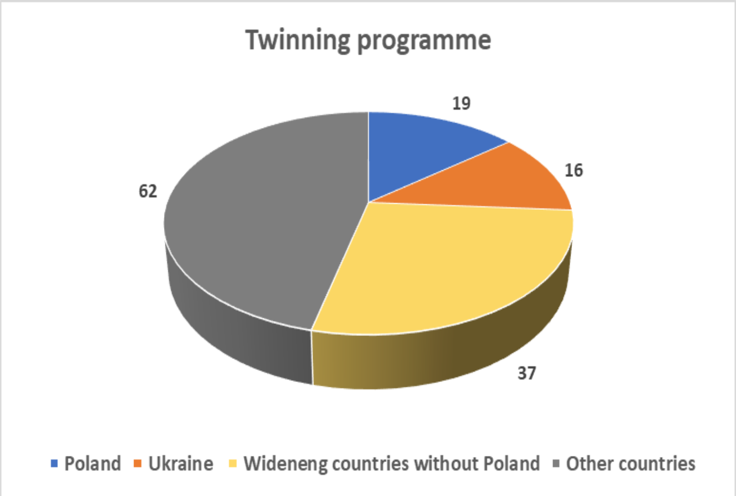


Figure 2. Number of users registered under the Twinning programme by country of affiliation

Early-Stage Researcher (ESR) Programme

The Early-Stage Researcher Programme is designed to support young, inexperienced scientists at an early stage of their academic careers. Through gaining hands-on experience at large-scale RIs, participants broaden their knowledge of various research techniques and their applicability across different scientific fields.

Under the ESR Programme, 16 partner RIs within the NEPHEWS project offer short, one-week internships. Participants receive reimbursement for travel and accommodation expenses related to their visits.

Initially, the programme was intended to support 24 young researchers; however, due to high interest, a total of 38 ESRs will ultimately receive support, including 9 affiliated with institutions in Poland (*Fig. 3*). This programme provides an important stepping stone for the next generation of scientists entering the field of photon and neutron research.

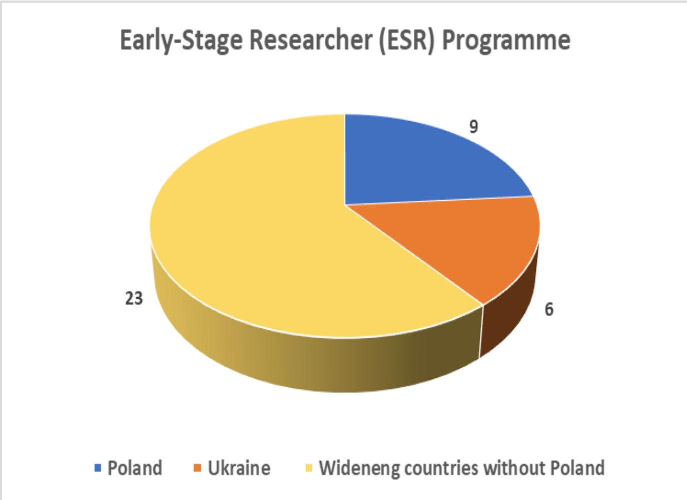


Figure 3. Number of ESR granted the internship under the ESR programme by country of affiliation

In addition to on-site user support, the NEPHEWS project offers virtual training sessions, enabling researchers from around the world to explore the opportunities provided by RIs. Recordings from previous sessions are available on the project's YouTube channel and website.

Summary

NEPHEWS is a landmark project whose strategic vision is grounded in the long-term strengthening of the European Research Area. Through reducing barriers to access advanced RIs, enhancing research capacity in less-resourced regions and supporting scientific mobility, NEPHEWS actively assists users of various scientific communities, and by promoting collaboration between neutron and photon communities it strengthens cooperation among different academic environments.

The project also fosters dialogue with national funding authorities to ensure sustainable access to large-scale research infrastructures beyond the project lifetime.

Additional information: More information about the NEPHEWS project, its ongoing activities, announcements, and opportunities to participate in access programmes can be found on the official website and on the project's LinkedIn profile.

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Visit of the ESRF representatives at IF PAN

Dr. Anna Wolska and MSc. Anna Reszka

Institute of Physics of the Polish Academy of Sciences, Warsaw, Poland

On 10–11 February, the Institute of Physics of the Polish Academy of Sciences (IF PAN) hosted a delegation from the European Synchrotron Radiation Facility (ESRF), one of the world's leading research infrastructures. The delegation included ESRF Director General Prof. Jean Daillant, Scientific Director Prof. Michael Krisch, and the ESRF Ambassador to Poland, Dr. Maciej Jankowski. The visit was organized by Dr. Anna Wolska (Polish delegate to the ESRF Council) and MSc. Anna Reszka (Polish delegate to the Administrative and Finance Committee, AFC).

The purpose of the visit was to extend cooperation between ESRF and IF PAN within the framework of the project "Polish Contribution to the European Synchrotron Radiation Facility," funded by the Ministry of Science and Higher Education. The project is coordinated by IF PAN on behalf of a National Cf\onsortium of *Scientific Institutions Interested in the Use of the European Synchrotron Radiation Source ESRF*. The project's implementation is possible thanks to the involvement of Dr. Anna Wolska, MSc Anna Reszka, and MSc Joanna Libera, project secretary.

The event also provided a platform to showcase ESRF research opportunities to the Polish scientific community and to discuss the framework of a new five-year cooperation project currently under preparation. The current arrangement, valid until the end of 2026, was signed on the first day of the meeting.

https://www.ifpan.edu.pl/en/current/news/visit-of-esrf-representatives-at-if-pan.html

In the afternoon, an open mini-symposium entitled *"Poland @ ESRF: Research and Perspectives"* was held. The event focused on ESRF research opportunities and the future development of the Polish synchrotron user community. ESRF representatives presented the facility's capabilities, including access to 46 beamlines supporting both fundamental and applied research in physics, chemistry, molecular biology, materials science, and related fields. A comprehensive suite of techniques is available, including diffraction, absorption, scattering, and imaging.

Prof. Jakub Szlachetko, Director of the National Synchrotron Radiation Centre SOLARIS, presented the current status and development plans of the Polish synchrotron. Prof. Agnieszka Witkowska, President of the Polish Synchrotron Radiation Society, outlined the history and future perspectives of the Polish synchrotron users community.

The final session was devoted to presentations by Polish ESRF users. Dr. Karolina Jurkiewicz (University of Silesia in Katowice) discussed studies on the local structure of amorphous molecular compounds under high-pressure. Prof. Maciej Kozak (Adam Mickiewicz University in Poznań) presented research on biomolecules under pressure. Prof. Beata Bochentyn (Gdańsk University of Technology) reported on catalytic properties of oxide cell materials studied at both SOLARIS and ESRF, highlighting the complementarity of the two facilities. The event was attended by representatives of Polish research institutions and members of the synchrotron user community.

On the second day, representatives of the ESRF and IF PAN met with Prof. Maria Mrówczyńska, Undersecretary of State, and representatives of the Ministry of Science and Higher Education. The discussions focused on ESRF's scientific potential, the activity of Polish research teams, and Poland's continued involvement in the development of this international research infrastructure.

https://www.ifpan.edu.pl/en/current/news/visit-of-esrf-representatives-at-if-pan.html

Poland joined the ESRF Consortium in 2004 as an associate member, initially contributing of 0.6% ESRF annual budget and, since 2006, 1%. This participation has been made possible through funding from the Ministry of Science and Higher Education. [1] As a result, Polish scientists can apply for a beamtime by submitting research proposals outlining planned experiments and expected outcomes. Proposals are evaluated solely on scientific merit by international Scientific Review Committees composed of experts in the relevant fields. Once approved, users receive comprehensive support from the ESRF. Beamline scientists prepare the experimental setup according to the proposal and ensure smooth operation of the instrumentation. ESRF also covers travel and accommodation costs for up to three researchers conducting the experiment. Calls for proposals are held twice a year, with deadlines on March 1 and September 10.

Publications and conference presentations resulting from ESRF experiments must acknowledge the funding supporting Poland's access to the facility, for example: "*The access to the ESRF was financed by the Polish Ministry of Education and Science, dec. no. 2021/WK/11.*"

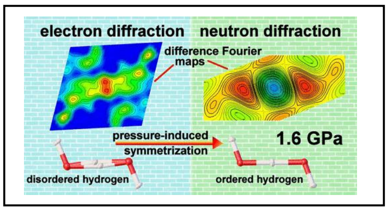
More information is available at: https://esrf.ifpan.edu.pl/

[1] Anna Wolska and Krystyna Ławniczak-Jabłońska *"Polish contribution to the European Synchrotron Radiation Facility"* Bulletin of the Polish Synchrotron Radiation Society 23 (2023) 8

The pictures can be found on the website (with the permission of Anna Wolska):

https://www.ifpan.edu.pl/en/current/news/visit-of-esrf-representatives-at-if-pan.html

Mechanism of Quantitative Changes in Electron Density in Natrochalcite during Pressure-Induced Hydrogen-Bond Symmetrization



Introduction. In the present study (P. Rejnhardt*, R. Gajda, M. Woińska, J. Parafiniuk, G. Giester, R. Miletich, Y. Wu, T. Poręba, M. Mezouar, Sz. Sutuła, T. Góral, P. Dera, K. Woźniak*, *Symmetrization of Strong Hydrogen Bond under High Pressure in Bihydroxide-Ion-Containing $NaCu_2(SO_4)_2{\cdot}H_3O_2$ Revealed by Experimental Charge Density, Single-Crystal Electron Diffraction, and Neutron Diffraction Studies*, **Journal of the American Chemical Society, 147(30) (2025) 2683–26843**, PMCID# PMC12314919, https://doi.org/10.1021/jacs.5c08310, we undertook a detailed investigation of the mechanism of strong hydrogen-bond symmetrization under high-pressure conditions, using the mineral natrochalcite, $NaCu_2(SO_4)_2{\cdot}H_3O_2$, as a model system. This mineral contains the bihydroxide anion $H_3O_2^-$, which hosts one of the shortest and strongest hydrogen bonds known in inorganic systems.

Hydrogen-bond symmetrization - defined as the disappearance of asymmetry between the proton donor and acceptor - is a fundamental problem in solid-state chemistry and geophysics. This process plays a crucial role in determining the physical properties of hydrous minerals, including their compressibility, proton conductivity, and capacity for water transport in the deep Earth mantle. Despite numerous theoretical and spectroscopic studies, the detailed mechanism has remained insufficiently understood, largely due to experimental limitations, particularly in accurately locating hydrogen atoms.

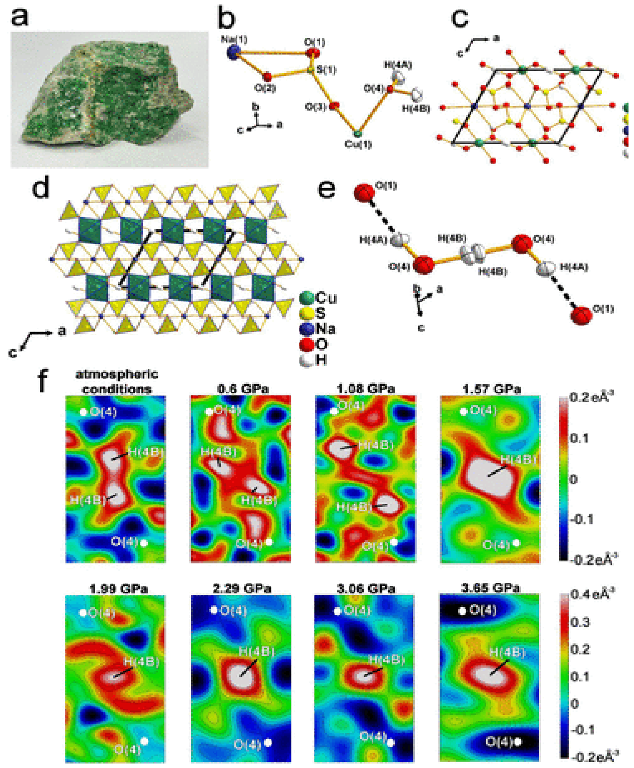


Fig. 1. Crystal structure of natrochalcite and residual Fourier electron density maps at various pressure conditions. (a) Sample of natural natrochalcite from Chuquicamata mine, Antofagasta, Chile. (b) Asymmetric unit of the natrochalcite crystal structure at RT conditions. (c) Atomic arrangement within the unit cell at RT conditions. (d) Projection of the polyhedral model of the natrochalcite structure at RT conditions along the Y-direction. (e) Bihydroxide ion in the structure of natrochalcite at RT conditions forming two HBs: shorter O(4)–H(4B)···O(4) with disordered hydrogen atoms and longer O(4)–H(4A)···O(1) H-bond. (f) Residual Fourier electron density maps calculated using the aspherical model of atomic electron density without the key hydrogen atom (H4B).

The aim of this work was therefore to directly track quantitative structural and electron-density changes within the O–H···O bonding system as a function of increasing pressure.

Methodology. To achieve this goal, we employed a complementary experimental approach combining:
-high-pressure single-crystal X-ray diffraction in diamond anvil cells, coupled with quantitative experimental electron-density analysis, -neutron diffraction, enabling precise localization of hydrogen atoms, -high-resolution electron diffraction. The latter two methods were used to validate the X-ray results.

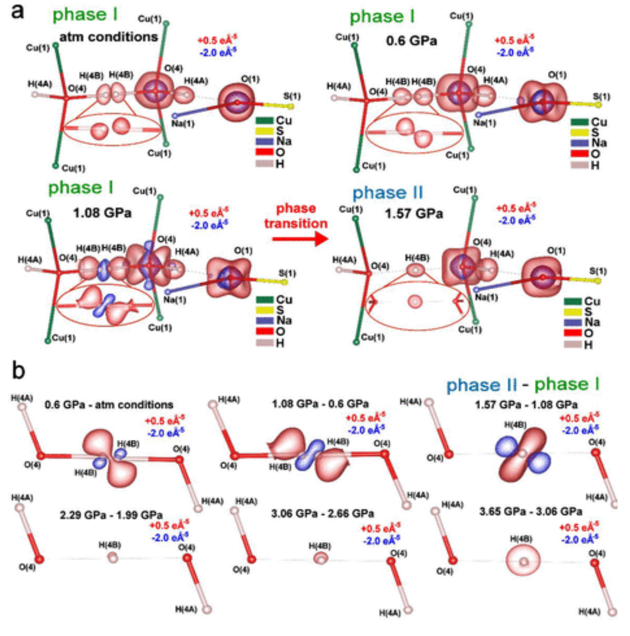


Fig. 2. (a) 3D maps of the negative Laplacian in the key hydrogen bond, (b) 3D maps of differences in the Laplacian of electron density when transitioning from lower to higher pressure. The isosurfaces are defined in the figure.

A key aspect of our methodology was the use of aspherical atomic electron-density models and refinement of the multipole electron density model in this mineral as a function of pressure. These approaches allow detection of subtle changes in electron distribution that are inaccessible within the conventional Independent Atom Model (IAM). Additionally, Hirshfeld Atom Refinement (HAR) was applied to validate the obtained geometric parameters.

The primary high-pressure X-ray diffraction data were collected at beamline ID27 of the European Synchrotron Radiation Facility (ESRF, Grenoble). Neutron measurements were performed at Oak Ridge National Laboratory (USA), while electron diffraction experiments were conducted using a Glacios electron microscope at the University of Warsaw.

Crystal Structure of Natrochalcite. The crystal structure of natrochalcite (Fig. 1) consists of chains of CuO_6 octahedra interconnected with SO_4 tetrahedra and coordination polyhedra surrounding sodium ions,
forming a three-dimensional network. A key structural feature is the presence of $H_3O_2^-$ anions forming extremely short hydrogen bonds, with a donor - acceptor distance of approximately 2.445 Å under ambient conditions. At ambient pressure and room temperature, the hydrogen atom involved in the central strong hydrogen bond is disordered over two equivalent positions related by inversion symmetry, indicating a double-well potential characteristic of an asymmetric hydrogen bond. Evolution of this bond with pressure is illustrated in Fig. 1f.

Mechanism of Hydrogen-Bond Symmetrization. Our results clearly demonstrate that increasing pressure induces a gradual and complex evolution of the hydrogen-bonding system, leading to symmetrization (Fig. 2). The process proceeds through several stages:

1. **Phase I (low pressure)**: The hydrogen atom remains disordered between two positions, and the hydrogen bond is asymmetric.
2. **Intermediate stage (~1.08 GPa)**: Protons shift toward the oxygen atoms and deviate from the O···O axis, indicating significant changes in local interactions.

3. **Phase II (≥ 1.57 GPa):** Then full symmetrization occurs - the proton localizes at the midpoint between the oxygen atoms, and the system becomes homogeneous.

Notably, symmetrization occurs at relatively low pressures (*ca.* 1.1 - 1.6 GPa), making this system exceptional among inorganic compounds.

Nature of the Phase Transition. Analysis of the pressure dependence of the unit-cell volume indicates that the symmetrization process corresponds to a second-order phase transition. No change in crystal symmetry is observed; the space group remains unchanged. The high-pressure phase with symmetric hydrogen bonds exhibits a higher bulk modulus, indicating increased structural rigidity.

Electron-Density Changes. A major achievement of this work is the direct observation of electron-density redistribution accompanying hydrogen-bond symmetrization. These changes were analyzed using:

- residual electron-density maps (Fig. 1f),
- the negative Laplacian of electron density distributions, where positive values (red) indicate regions of electron concentration and negative values (blue) indicate depletion (Fig. 2a),
- difference maps of the negative Laplacian between successive pressure points (Fig. 2b).

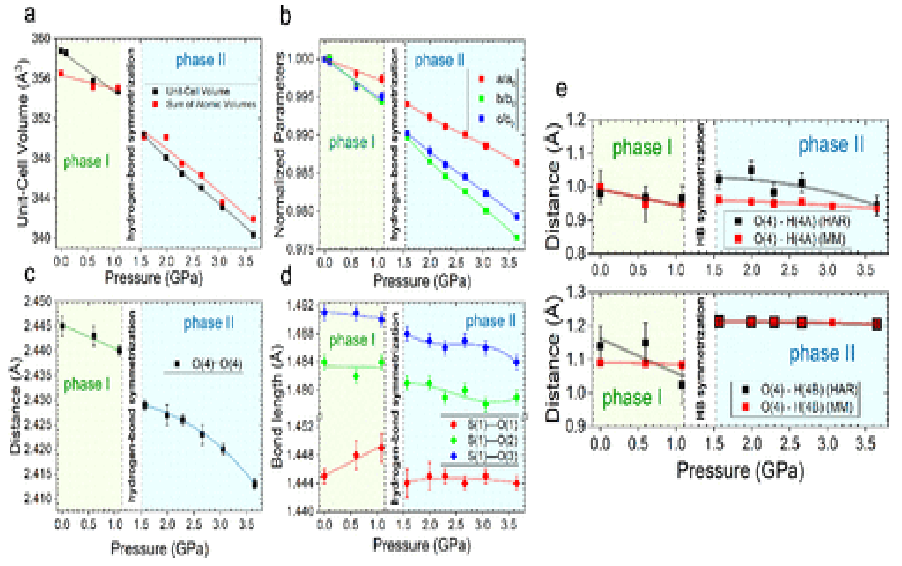


Fig. 3. Changes in selected structural and electronic parameters as a function of pressure: (a) variation of the unit-cell volume (and the sum of atomic volumes), (b) variation of normalized unit-cell parameters, (c) change in the O(4)···O(4) distance, (d) changes in other bond lengths (S–O), as well as variations in bond lengths involving hydrogen atoms.

The latter provide the most sensitive descriptor of electron-density evolution. Red regions indicate accumulation of electron density in the hydrogen bond upon compression, while blue regions indicate depletion. Between 1.08 GPa and 1.57 GPa, a complete reversal of electron-density polarization occurs prior to bond symmetrization. Only after this redistribution does electron density accumulate symmetrically at the bond center, increasing further with pressure.

In summary:

- **Low-pressure phase:** electron density is depleted at the bond center and concentrated near oxygen atoms.
- **Near transition:** abrupt redistribution toward the bond center occurs.
- **Symmetric phase:** maximum electron density coincides with the proton position, and the bond becomes more uniform.

These results indicate that hydrogen-bond symmetrization is associated with significant bond strengthening and partial covalent character.

Variation of Atomic Parameters. The applied methods enabled not only determination of structural parameters (e.g., interatomic distances) (Fig. 3) but also changes in unit-cell parameters, atomic charges, and atomic volumes. A key result is the decomposition of the macroscopic equation of state (V = f(P)) into atomic equations of state (Vatom = f(P)), demonstrating that atoms exchange electron density as a function of pressure which is supported by illustrations in Fig. 3.

Verification by Neutron and Electron Diffraction. Neutron diffraction unambiguously confirmed the central position of the proton in the high-pressure phase. Fourier maps revealed a single maximum (minimum for neutrons) at the bond center, excluding dynamic disorder (Fig. 4).

Electron diffraction allowed observation of subtle effects related to hydrogen-position splitting at low pressure and provided insight into temperature-dependent structural behavior.

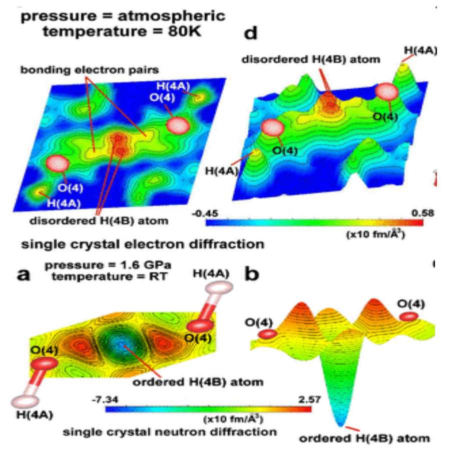


Fig. 4. Illustration of the key hydrogen bonding determined by electron diffraction (upper panel) and neutron diffraction (lower panel).

Significance of the Results. These findings have important implications for: **geophysics**, particularly water transport in the Earth's mantle; **materials chemistry**, especially systems with strong hydrogen bonds, **high-pressure physics**, including proton conductivity and superconductivity.

We demonstrate that hydrogen-bond symmetrization is governed by subtle changes in electron-density distribution rather than purely geometric parameters.

Conclusions. In this work, we:

- performed the first comprehensive analysis of hydrogen-bond symmetrization based on experimental electron density under high pressure results,
- demonstrated that the process occurs at exceptionally low pressure in natrochalcite,
- identified the mechanism of electron-density special redistribution responsible for the H-bond transformation,
- confirmed the transition from predominantly electrostatic to partially covalent bonding character.

Our results significantly advance the understanding of strong hydrogen bonds and the behavior of matter under extreme conditions. The work was highlighted by the ESRF (*ESRF Spotlight on Science*): https://www.esrf.fr/home/news/spotlight/content-news/spotlight/charge-density-mapping-reveals-hydrogen-bond-symmetrisation-in-natrochalcite-under-high-pressure.html and 2. Oak Ridge National Lab (ONRL, USA), https://neutrons.ornl.gov/highlights/summarization-strong-hydrogen-bond-under-high-pressure-bihydroxide-ion-containing

The paper also contains many other interesting results, and we encourage readers to consult the original publication.

Acknowledgements. We acknowledge the European Synchrotron Radiation Facility (ESRF) for access to synchrotron infrastructure (project ES-1296), funded by the Polish Ministry of Science and Higher Education (decision no. 2021/WK/11). The neutron-scattering component utilized resources of the High Flux Isotope Reactor (HFIR), a DOE Office of Science User Facility operated by Oak Ridge National Laboratory (USA), with measurements performed on the DEMAND instrument (project IPTS-32868.1). This work was supported by the National Science Centre, Poland (OPUS grant UMO-2019/33/B/ST10/02671 awarded to K.W.). The research was conducted at the TEAM TECH Core Facility (Centre of New Technologies, University of Warsaw), funded by the Foundation for Polish Science.

Invitation. We invite readers to take advantage of advanced structural studies of even nanocrystals using electron diffraction on the Glacios electron microscope at the Center for New Technologies of the University of Warsaw.

Prof. dr hab. Krzysztof Woźniak, Wydział Chemii UW, e-mail: kwozniak@chem.uw.edu.pl

Effect of high-pressure on the structure of "amorphous" pharmaceuticals with flexible molecules

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In April 2025, Anna Janowska, a second-year student in Physics at the University of Silesia in Katowice, completed a Master internship at the European Synchrotron Radiation Facility (ESRF). Access to the ESRF was financed by the Polish Ministry of Science and Higher Education – decision no. 2021/WK/11.

During the internship, I conducted research whose results were incorporated into my master's thesis. The internship topic was: "Effect of high pressure on the supramolecular structure of pharmaceuticals in amorphous-like states". During the internship, I had an opportunity to conduct high-pressure diffraction measurements of active pharmaceutical ingredients (APIs) in collaboration with Dr. Gaston Garbarino, scientist responsible for the High Pressure Laboratory at ESRF. The high-pressure X-ray diffraction experiment in a diamond anvil cell (DAC) was successfully performed at ID15B beamline, which is dedicated to the determination of structural properties of solids at high pressure using angle-dispersive diffraction with DACs. We used DACs to melt the pharmaceutical compounds under high-pressure conditions, up to hundreds of MPa. These are the compaction pressures used in the pharmaceutical industry for tableting.

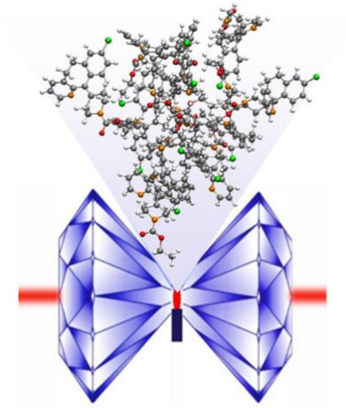


Figure 2 A schematic representation of a DAC.

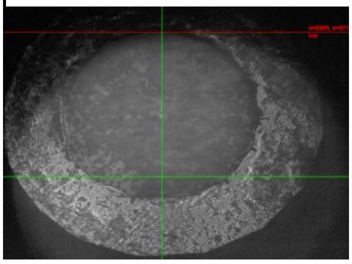


Figure 1 A sample in a DAC.

We aimed to identify changes in the local structure of pressurized liquids and to predict whether the properties of glasses produced by the vitrification of such liquids may be inherited from their liquid precursors. The research conducted is currently not feasible using laboratory diffraction techniques.

The study of the effect of high pressure on the structure of amorphous pharmaceuticals is a "hot" topic because it addresses the core challenge of physical stability during pharmaceutical manufacturing (such as tableting), where high pressures are routinely applied. While amorphous forms in the glassy states are desired to enhance the bioavailability of poorly soluble compounds that are available in stable crystalline forms, they are metastable and tend to recrystallize, losing their effectiveness. Producing pressure-densified glasses (PDGs) involves applying high pressure to glass-forming liquids at elevated temperatures to force higher-density structural states that may be maintained upon cooling and pressure release. Such PDGs usually exhibit greater solubility than their ordinary glasses (OGs), which are produced by the vitrification of liquids at ambient conditions. However, the microscopic structural origin of differences between PDGs and OG remains unclear.

The research for my master's thesis focused on the structure of two substances that represent a class of APIs composed of flexible molecules – probucol and loratadine (*Figure 3*). Previous studies employing broadband dielectric spectroscopy conducted by scientists from the University of Silesia had indicated changes in the molecular dynamics of these APIs under high-pressure conditions [1,2]. My aim was to determine the origin of the changes – whether they are intra- or intermolecular. The studies were supported by molecular dynamics simulations consistent with experimental diffraction data. The results showed that structural changes occurring as a result of the application of elevated pressure are primarily driven by compression-induced decrease in volume. This is especially the case of loratadine, in the system of which a tendency of clustering of chlorine atoms was observed (see *Figure 4b*).

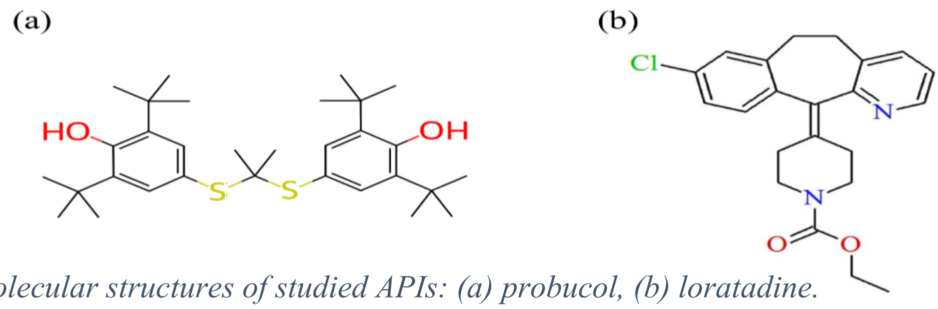
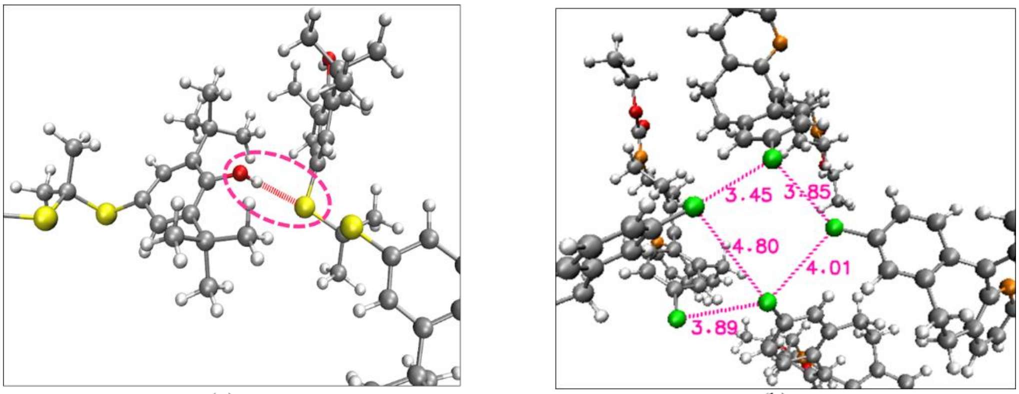


Figure 3 Molecular structures of studied APIs: (a) probucol, (b) loratadine.

Specifically, the effect of high pressure was similar to that of cooling. However, in the case of probucol, high pressure affects the packing of molecules, particularly the sulfur-sulfur arrangement, and also increases the tendency to form weak O-H···S hydrogen bonds (Figure *4*Figure 4a). Based on the result obtained, a scientific paper is being prepared.



(a) (b)

Figure 4 Examples of intermolecular organization in compressed systems of (a) probucol - weak O-H···S hydrogen bonding, (b) loratadine - clustering of chlorine atoms.

We remind that students with polish affiliations, preparing to write their master's thesis can still apply for an internship at the ESRF. The internship can last up to six months. During this time, the student can conduct research or participate in creating codes for data analysis. The results obtained should be incorporated into the master's thesis. More information about internships and research at the ESRF, which can be fully funded by a grant from the Ministry of Science and Higher Education (Decision No. 2021/WK/11), can be found on the website: https://esrf.ifpan.edu.pl/.

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Oscillating structural transformations in the electrochemical synthesis of graphene oxide from graphite

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Electrochemical oxidation of graphite in aqueous inorganic acids is known to occur with potential oscillations [1, 2], however the structural changes underlying these oscillations have remained unclear. Structural studies performed using in situ time-resolved synchrotron X-ray diffraction (XRD) during anodic oxidation of graphite in aqueous sulfuric acid reveal that the periodic potential oscillations correlate with the appearance and disappearance of a solid phase identified as stage-1 graphite intercalation compound (GIC). The gathered results provide broad insights into the oscillating structural changes occurring during the anodic graphite oxidation in aqueous H_2SO_4 and allow for an update of the mechanism of graphite oxide (GO) electrochemical formation [3].

A microscopic capillary-sized electrochemical reactor was designed and successfully implemented to identify all the intermediate phases formed within cycles of potential oscillations, occurring during the electrochemical graphite oxidation in 11 M H_2SO_4 (Fig. 1). The experiment was performed at ESRF beamline ID22, which is specialized in high resolution powder diffraction experiments. High-quality XRD pattens can be gathered periodically in a short period of time which allows to observe step-by-step the structural changes of graphite during its electrochemical oxidation in aqueous H_2SO_4 solution in relatively complex electrochemical cell. This would not be possible with

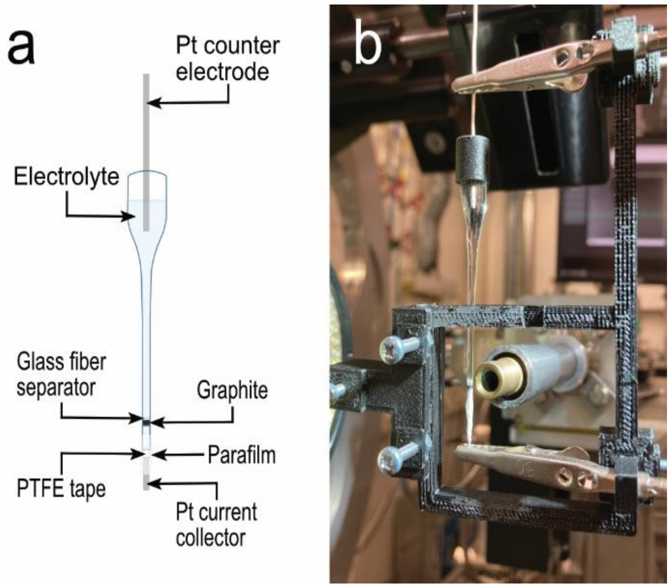

Figure 1. a) Scheme of the micro-electrochemical reactor. b) Photo of the installed reactor aligned in synchrotron radiation beam and connected to the potentiostat-galvanostat.

conventional XRD aperture. Structural studies performed in situ directly during the process of electrochemical oxidation are required to reveal the fundamental mechanism of graphite electrooxidation. Synchrotron radiation XRD patterns were recorded in transmission mode every 1 minute to study the mechanism of electrochemical transformation of graphite into GO. The heat map constructed of XRD patterns recorded every minute during graphite electrooxidation combined with recorded galvanostatic curve is presented in Fig. 2. Firstly, the voltage between graphite and platinum increases continuously and the formation of stage-2 GIC occurs (stage-*n* is defined as the *n* number of graphene layers between neighboring intercalated layers). Next, when the charge density of 200 C g^{-1} is reached, the voltage starts to oscillate. According to the earlier published models (mostly based on ex situ experiments), a gradual step-like transformation of stage-2 GIC into pristine graphite oxide (PGO) could be expected during the reaction [2, 4]. Surprisingly, XRD detected the formation of stage-1 H_2SO_4-GIC with an interlayer spacing of 7.8 Å. After some time, the voltage suddenly drops and the intensity of (002) reflection assigned to the stage-1 GIC decreases during the voltage drop until it disappears completely. Next, the voltage starts to increase, until it reaches the voltage wave maximum, where another part of stage-2 GIC is transformed into stage-1 GIC. Appearance and disappearance of stage-1 GIC occur periodically with the maximum and minimum of voltage oscillations, respectively. When the charge ~1300 C g^{-1} is reached, the signal originating from PGO with an interlayer spacing of 14.2 Å appears and its intensity increases over time. On the other hand, the intensity of stage-2 GIC (002) reflection is decreasing during the graphite transformation into PGO and when the process is finished, the signal from stage-2 practically disappears.

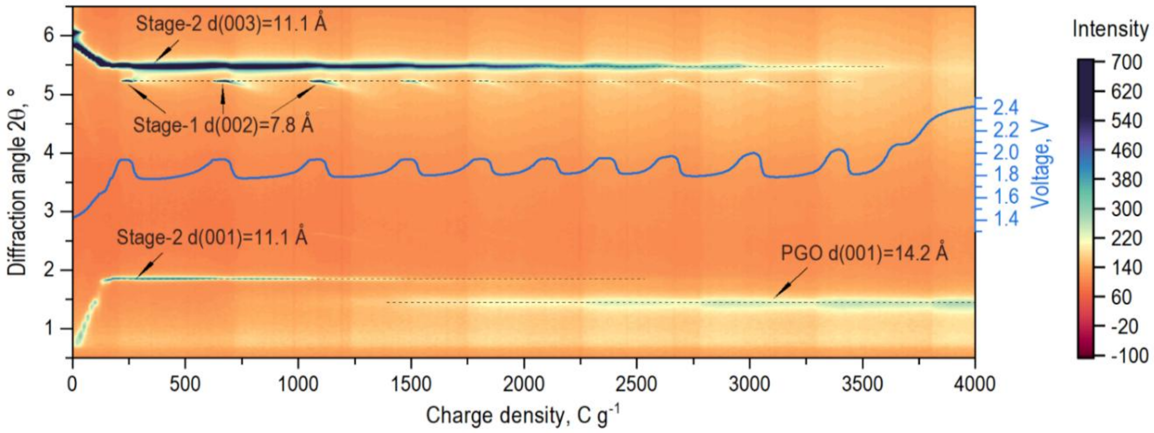

Figure 2. Heat map constructed using XRD patterns (λ=0.35435 Å) recorded during the electrochemical graphite oxidation combined with the galvanostatic curve showing voltage oscillations.

The transformation from stage-2 GIC into PGO occurs not as a continuous change, but through oscillations, as competition between two reactions:

1. Stage-2 GIC to stage-1 GIC conversion, which occurs in 11 M H_2SO_4 only at higher voltage.
2. Conversion of stage-1 GIC into PGO which requires lower voltage.

The number of oscillations, the oscillation frequency, and the potential amplitude are strongly affected by the concentration of sulfuric acid (proportion between amount water and sulfuric acid in the solution) [2].

The reaction studied here has features similar to the oscillating reactions: non-equilibrium conditions, a source of external energy provided by a constant electrical current, the presence of two competing reactions and periodic changes in the composition of the system. However, the periodic appearance and disappearance of the solid phase with a certain well-defined structure found in our experiments seem to represent a completely new feature not found in "classical" oscillating reactions.

Full article describing in detail the electrochemical transformation of graphite into graphite oxide is published in Angewandte Chemie journal [3].

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MAVKA – microfocus X-ray spectroscopy beamline at SOLARIS synchrotron

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Construction of MAVKA beamline at SOLARIS synchrotron is an ongoing project, initiated by the League of European Accelerator-based Photon Sources (LEAPS). This project, titled Light for Ukraine (L4U), aims to broaden research opportunities for Ukrainian scientific community, which were heavily impaired by the ongoing war, and promote the development of international collaborations between Ukrainian and European scientific institutions. In 2023, during the dedicated L4U workshop, an idea to construct a new beamline at SOLARIS synchrotron was proposed, with a goal to create a consolidation site for Ukrainian scientific community and share an expertise of operating and conducting research on a unique scientific instrument, which is synchrotron radiation facility [1]. Following the L4U workshop, a dedicated survey of Ukrainian scientists interested in synchrotron-based research was conducted. The survey highlighted that research which employs micro-/nano- X-ray spectroscopy is of the most interest to the Ukrainian scientific community, outlining the general beamline design strategy.

The construction of the MAVKA beamline is funded via donations of equipment or grant applications by the L4U project partners. The implementation of the L4U project was commenced after the initial 1.5 M CHF funding, granted to Paul Scherrer Institute (PSI) by the Swiss National Science Foundation (SNSF) and Swiss State Secretariat for Education, Research and Innovation (SERI). In addition, in the process of the Swiss Light Source (SLS) 2.0 upgrade, PSI has committed to contribute in-kind major beamline components. Complementarily, SOLARIS is partially funding the design and construction of MAVKA beamline and assumes the cost of operational expenses for the lifetime of the beamline. Consequently, an operational framework was proposed, which envisions formation of the international coordination group and distribution of MAVKA beamtime through SOLARIS calls. A significant percentage of beamtime will be exclusively allocated to the proposals submitted by the members of Ukrainian community.

The source for the MAVKA beamline is an in-vacuum U19 undulator, which will generate high flux radiation in a broad 0.5 - 12.0 keV energy range. Frontend of the MAVKA beamline is identical to the Swiss Light Source (SLS) 2.0 upgrade frontend produced by PSI [2], with minor modifications necessary to account for the SOLARIS synchrotron ring parameters. The designed frontend consists of X-ray beam position monitor (XBPM), high-power diaphragm, photon shutter, beam stopper and high-power slits, ensuring proper shaping and alignment of the beam for the downstream beamline components.

Optical layout of the MAVKA beamline includes attenuators module, bendable toroidal mirror (M1), double-crystal monochromators (DCM), XBPMs, slits and safety shutter (Figure 1). These components will be installed in the first stage of the beamline construction and enable operation in the tender-to hard X-ray energy range (2.5 - 12 keV). Second stage of the construction envisions installation of the plane grating monochromator (PGM) and corresponding exit slits, in order to facilitate operation in the soft X-ray energy range (0.5 - 2.5 keV). Focusing of the beam on the endstations sample position will be handled by the dedicated Kirkpatrick–Baez (KB) mirror systems. The minimum beam size at the sample position is expected to be in the 1 - 50 μm range (depending on the endstation), with the flux of up to 10^{12} photons/s.

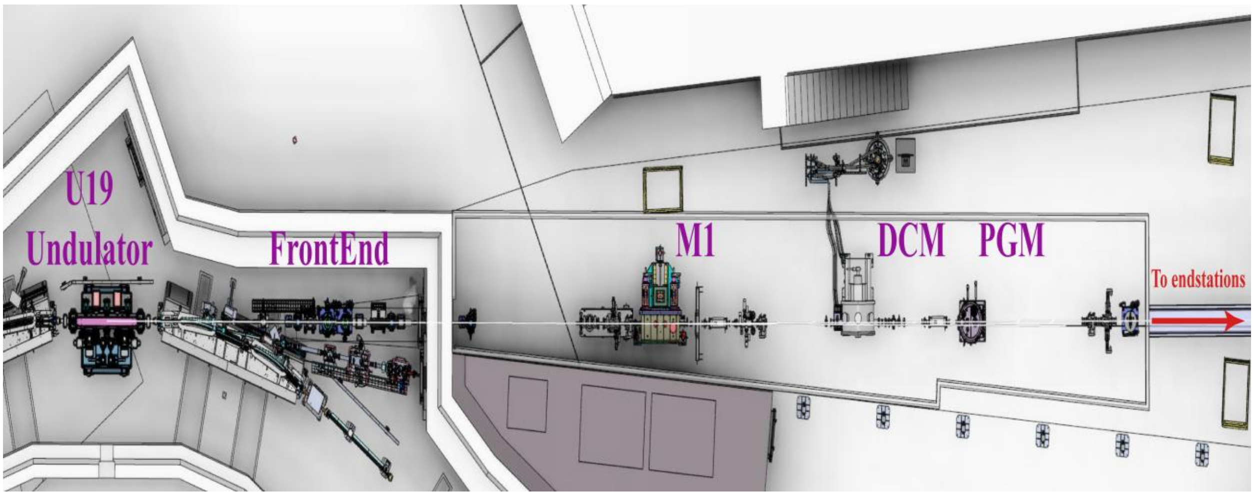

Figure 1. Layout of the MAVKA beamline. The endstations design is a work in progress.

MAVKA beamline is envisioned to host three endstations in the experimental hutch (Figure 1). First, an X-ray photoelectron spectroscopy endstation (XPS) will be dedicated to high-resolution studies of the electronic structures of surfaces and interfaces, with a beam spot size below 50 μm. Second, an ambient pressure hard X-ray photoelectron spectroscopy (AP-HAXPES) endstation, equipped with “dip and pull” and liquid jet modules, will enable in-situ/operando studies of the electrochemical processes. Options for a third endstation, capable to achieve a beam spot size as small as 1 μm, are currently under consideration. This endstation will be aimed at high resolution X-ray spectroscopy/scattering studies in the tender-hard X-ray range. Combined, these three endstations will provide a comprehensive set of methodologies for studies in electronics, catalysis, electrochemistry, biomedicine, etc.

Current timeline envisions completion of the first stage of beamline construction and beginning of commissioning of optical components by the end of 2027. However, the timeline of commissioning of endstations and start of user operation is not yet defined, as L4U project partners are still in the process of sourcing funding for the beamline endstations.

In conclusion, MAVKA beamline is being constructed with a goal to provide Ukrainian scientific community with an access to unique research tools and to create a supportive environment that promotes collaborations and exchange of expertise and ideas. We believe that it can become a stepping stone towards the recovery and prosperity of Ukrainian science.

Acknowledgements:

The MAVKA project team involves representatives from National Academy of Sciences of Ukraine (Alexander Kordyuk, Volodymyr Bezguba, Volodymyr Karbivskyy, Ihor Sukhenko, et al.), SOLARIS National Synchrotron Radiation Centre (Jakub Szlachetko, Michał Młynarczyk, Marcin Sikora, Marcin Zając, Anna Wach, Adriana Wawrzyniak, Jarosław Wiechecki, Andrzej Marendziak, Paweł Bulira, Paweł Nowak, et al.), Paul Scherrer Institute (Luc Patthey, Leonid Rivkin, Danylo Babich, Rolf Follath, Marco Calvi, David Marco Just, Daniel Grolimund, Marcel Brüstle, et al.), Deutsches Elektronen-Synchrotron (Wolfgang Drube, Andrei Hloskovsky, Oksana Chukova, Martin Sandhop, et al.).

The project team gratefully acknowledges the CHF 1.5 million grant from the Swiss State Secretariat for Education, Research and Innovation (SERI) and the Swiss National Science Foundation (SNSF).

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Ultrafast two-colour XES unravels details of the excited states in base metal dyads for photocatalytic proton reduction

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The growing demand for sustainable energy technologies has intensified the search for alternatives to noble-metal-based catalysts. Photocatalytic water splitting represents a particularly attractive route toward clean hydrogen production, offering a sustainable alternative to currently used approaches. A key challenge in this field is the design of catalytic systems that efficiently harvest solar energy and direct it toward chemical bond formation.

Bimetallic molecular assemblies, commonly referred to as dyads, are promising platforms for the direct conversion of sunlight into chemical energy carriers such as hydrogen. However, replacing noble metals with earth-abundant elements remains challenging. One of the main obstacles is the still incomplete understanding of the working principles that govern heterobimetallic base-metal complexes, which currently limit their catalytic efficiency. Therefore, detailed insight into their excited-state dynamics and charge-transfer pathways is essential for the rational design of improved photocatalytic systems. The prototypical system investigated here consists of an Fe(II)-based photosensitizer covalently linked to cobaloxime, a cobalt-based water-reduction catalyst. Upon photoexcitation, the Fe(II) N-heterocyclic carbene complex acts as the light-harvesting unit,

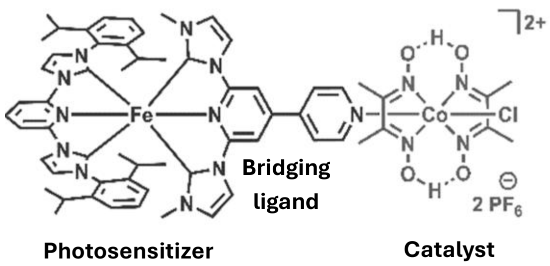

Fig. 1 The molecular structure of the dyad

while electron density is transferred through a bipyridine bridging ligand toward the Co(III) center of the cobaloxime moiety. Initial characterization showed that this dyadic architecture doubles the H_2 production efficiency compared with the corresponding two-component system.

The earliest events following photoexcitation — namely excited-state formation and photoinduced electron transfer from the photosensitizer to the catalyst — determine the activity of dyads in photocatalytic reduction reactions. These processes originate from non-equilibrated states in the Franck–Condon region, where conventional analytical approaches are often insufficient to directly connect electronic dynamics with molecular structure.

To address this challenge, we employed femtosecond time-resolved X-ray emission spectroscopy at the European XFEL to track electronic and structural dynamics in the bimetallic assembly under catalytic conditions. Because the relevant processes occur on ultrafast timescales and involve both partially unknown excited states at the iron photosensitizer and optically dark states at the cobalt catalyst, a two-colour X-ray emission (XES) experiment was implemented. This approach enabled the simultaneous detection of Fe and Co Kα emission lines, eliminating ambiguities related to time-zero determination and allowing the ultrafast excited-state dynamics to be directly correlated with electron-transfer processes within the dyad.

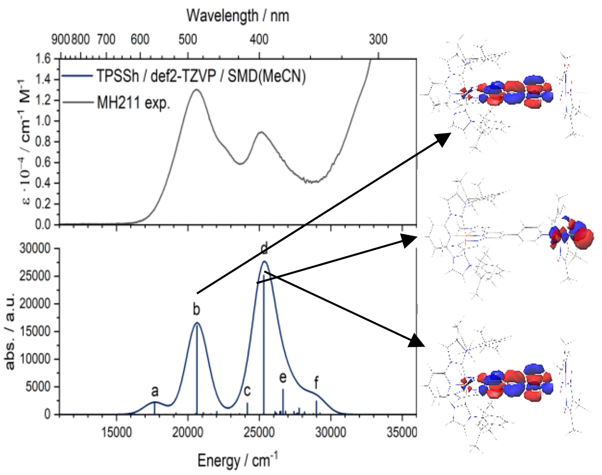

Fig. 2 UV-VIS measurements (top), TD-DFT interpretation (bottom) and selected charge-transfer orbitals obtained from the TD-DFT calculations (right).

In the two-colour XES experiment, Fe and Co emission signals were measured simultaneously with sub-picosecond time resolution at the FXE instrument of the European XFEL. The Fe–Co dyad was investigated as a 10 mM solution delivered through a cylindrical liquid jet with a diameter of 100 μm. The sample was excited at 400 nm using optical laser pulses with an energy of 3.4 μJ per pulse, corresponding to an excitation fraction of approximately 55%. The electronic configuration was probed using 9.3 keV X-ray pulses at a repetition rate of 0.564 MHz, with 125 bunches per pulse train. Data were collected in an energy-dispersive geometry using a 16-crystal von Hamos XES spectrometer coupled to a two-dimensional charge-integrating Jungfrau detector with a 1024 × 1024-pixel matrix. As references for the dyad measurements, the isolated cobalt catalyst fragment and the iron photosensitizer fragment were measured under identical experimental conditions. While

X-ray emission spectroscopy is highly sensitive to metal-centered states, it is less directly sensitive to charge-transfer states. Therefore, the X-ray measurements were complemented by femtosecond transient absorption spectroscopy in the visible range, which is particularly suited to monitoring metal-to-ligand charge-transfer states.

The ground-state UV–Vis spectrum revealed characteristic absorption bands, which were further assigned using TD-DFT calculations. Two prominent MLCT bands were identified around 400 and 495 nm. The band at approximately 400 nm also contains contributions assigned to metal-to-metal charge transfer. Transient absorption measurements following 400 nm excitation provided insight into the early evolution of the excited-state landscape. In both the isolated photosensitizer and the Fe–Co dyad, the dynamics are dominated by a long-lived MLCT state with a lifetime of approximately 10–15 ps, accompanied by an intermediate-lived metal-centered state and an ultrafast short-lived component. Pump–probe X-ray emission measurements confirmed the presence of the triplet MLCT state, the triplet metal-centered state, and an additional short-lived component with a lifetime of approximately 300 fs. Furthermore, nuclear wavepacket dynamics were observed in the Fe ΔXES signal for both the photosensitizer and the dyad. At the Co Kα emission line, the cobalt moiety of the dyad displayed an additional 250 fs time component compared with pure cobaloxime, along with a distinct spectral lineshape characteristic of a charge-transfer state. All spectral components were assigned with the support of multiplet calculations in octahedral ligand fields. Subsequent population analysis, based on analytical solutions of the corresponding differential equations, indicated that the triplet MLCT state acts as the electron donor for the additional charge-transfer component observed at the cobalt site. The simultaneous measurement of Fe and Co XES signals was crucial for this assignment, as it removed uncertainties associated with independent time-zero determination.

The combination of ultrafast pump–probe experiments in the X-ray and optical regimes provides a uniquely complementary view of the excited-state dynamics in complex bimetallic assemblies. The different sensitivities of X-ray emission and transient absorption spectroscopy enabled independent assignment of the MLCT state. In addition, vibronic oscillations that were not visible in the transient absorption data were clearly resolved by X-ray emission spectroscopy, pointing to their metal-centered origin.

The combined experimental and theoretical analysis allowed the nature and magnitude of charge transfer in the dyad to be evaluated. The observed charge-transfer efficiency was found to be only a few percent. This relatively low value can be rationalized by the structural flexibility of the bipyridine bridging ligand, which possesses several rotational degrees of freedom. In conjugated π-electron systems, efficient conductivity depends strongly on the overlap of their antibonding π* orbitals. The rotational motion of the bridge, also reflected in the observed vibronic oscillations, likely reduces this overlap and thereby limits the efficiency of electron transfer. These findings suggest a clear strategy for improving future dyad designs: immobilization of the central C–C bond within the bipyridine bridge could stabilize the overlap of the π* orbitals and enhance charge-transfer efficiency. Such structural control may provide a route toward more efficient base-metal photocatalysts for solar-driven hydrogen production.

Further details are available in the cited literature:

M. Huber-Gedert et al., Chemistry – A European Journal ***2021****, 27, 9905.*
M. Nowakowski et al., Advanced Science ***2024****, 11, 2404348*

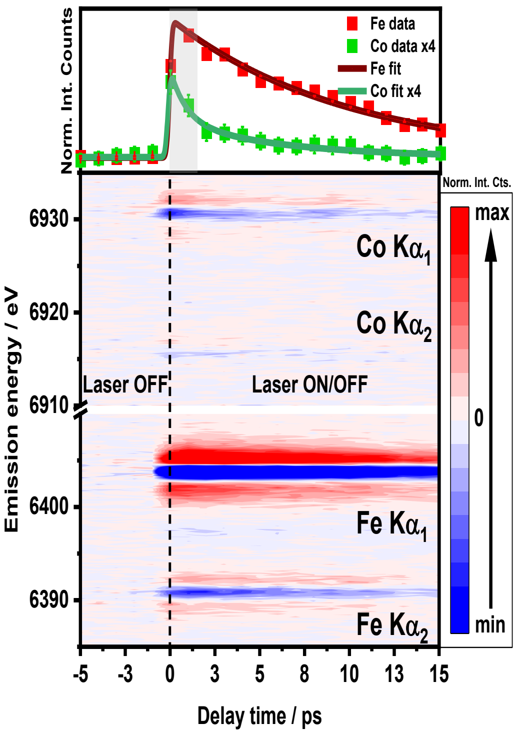

Fig. 3 Two-color femtosecond transient Kα XES data for the dyad. Top: Kinetic traces of the Fe (red) and Co (green) ΔXES integrated at respectively.

Electronic and Structural Relaxation of Photoexcited WO_3 Observed by Femtosecond Resonant X-ray Spectroscopy

The coupled electronic and structural relaxation pathways in photoexcited tungsten trioxide, WO_3, are studied using femtosecond resonant X-ray spectroscopy. By probing the system on ultrafast time scales, the work aims to resolve how photoinduced charge redistribution is connected to local structural changes around tungsten sites. The experiment provides element-specific insight into the early relaxation dynamics of a transition-metal oxide relevant to photocatalysis, electrochromic, and photoresponsive materials. The use of resonant X-ray methods enables sensitivity to both electronic-state evolution and changes in local coordination geometry. The research contributes to the broader understanding of ultrafast carrier–lattice coupling in functional oxide materials.

The Journal of Physical Chemistry Letters, DOI: 10.1021/acs.jpclett.5c01062

Attosecond X-ray Sources, Methods, and Applications at Present and Future Free-Electron Lasers: Tutorial

The tutorial article reviews the development of attosecond X-ray capabilities at current and next-generation free-electron laser facilities. It discusses the generation, characterization, synchronization, and application of ultrashort X-ray pulses for probing electron dynamics on their natural time scale. The paper provides a methodological and conceptual framework for attosecond science at XFELs. Particular emphasis is placed on pump–probe schemes, nonlinear X-ray interactions, and future opportunities for resolving charge migration, Auger decay, and correlated electron motion. The article is therefore best understood as a high-level reference for emerging attosecond XFEL spectroscopy.

Advances in Optics and Photonics, DOI: 10.1364/AOP.540527

Interpretable neural network predictions of high-intensity femtosecond x-ray free-electron laser pulses using sulfur K-shell emission spectra

The paper focuses on the use of interpretable neural-network models to predict material or atomic responses under intense femtosecond X-ray irradiation. It is highly relevant to XFEL experiments, where ultrashort pulses can induce nonlinear ionization, electronic rearrangement, and radiation-damage processes during or immediately after the probe event. The key focus is put not only predictive accuracy but also physical interpretability of the machine-learning model. This can help identify which experimental or microscopic parameters most strongly control the response to high-intensity X-ray fields. The work is relevant for understanding and modeling the conditions under which XFEL-based spectroscopy is performed

Physical Review Research, DOI: 10.1103/dwc6-7hvn

High gas-pressure apparatus for nonlinear X-ray propagation and reshaping via stimulated X-ray Raman scattering

The report presents an experimental apparatus designed for studying nonlinear X-ray propagation in gases under high-pressure conditions. Intense X-ray pulses can drive nonlinear light–matter interactions that are inaccessible with conventional synchrotron sources. The apparatus enables controlled studies of

X-ray pulse reshaping, absorption, propagation effects, and the interaction of modified XFEL pulses with secondary targets. It expands the experimental toolbox for nonlinear and high-field X-ray physics at XFEL facilities.

Scientific Reports, DOI: 10.1038/s41598-025-32245-x

Demonstration of Time-Resolved Fe K-edge XANES with a Self-Seeded X-ray Free-Electron Laser at PAL-XFEL

The paper demonstrates time-resolved Fe K-edge XANES using a self-seeded hard X-ray free-electron laser at PAL-XFEL. The use of self-seeding improves the spectral properties of the XFEL pulse compared with standard SASE operation, making XANES measurements more stable and spectroscopically informative. The study shows that time-resolved XANES can be implemented under XFEL conditions to follow ultrafast electronic or structural changes around iron centers. As a state-of-the-art experiment, the paper validates the feasibility of element-specific absorption spectroscopy with improved temporal and spectral resolution. It represents a direct and highly relevant example of XFEL-based XAS methodology.

Scientific Reports, DOI: 10.1038/s41598-025-32237-x

X-ray Absorption Spectroscopy of Dilute Metalloenzymes at X-ray Free-Electron Lasers

X-ray absorption spectroscopy is performed on dilute metalloenzyme samples at XFEL facilities. Biological metal centers often occur at low concentrations, while XFEL pulses exhibit strong shot-to-shot fluctuations that complicate normalization and signal recovery. The work demonstrates experimental strategies for acquiring reliable XAS data from low-concentration metalloprotein or metalloenzyme systems. It extends XFEL-based XAS toward biologically realistic samples, where sample quantity, radiation damage, and signal-to-noise limitations are major constraints. The article contributes for future time-resolved studies of enzymatic catalysis and metalloprotein function.

The Journal of Physical Chemistry Letters, DOI**:** 10.1021/acs.jpclett.5c00399

Femtosecond Soft X-ray Absorption Spectroscopy Identifies Metal-Centered S_1 Excited State of Cyanocobalamin

Femtosecond soft X-ray absorption spectroscopy is applied to determine the electronic character of the first excited singlet state, S_1, in cyanocobalamin. By probing core-level transitions associated with the metal center, the authors obtain element-specific information about the transient electronic structure following photoexcitation. The central conclusion is that the S_1 state has substantial metal-centered character, which is important for understanding the photophysics of vitamin B_{12} derivatives. The study illustrates the power of ultrafast XAS for distinguishing ligand-centered, charge-transfer, and metal-centered excited states in complex molecular systems. It is an example of how femtosecond X-ray spectroscopy can resolve electronic-state assignments that are difficult to access using optical spectroscopy alone.

Journal of the American Chemical Society, DOI**:** 10.1021/jacs.6c01860

Ultrafast Dynamics of Electronic and Structural Modifications Induced by Photoexcitation in Cerium Oxide

With pump-probe Ce L3-edge XAS, the research investigates ultrafast electronic and structural response of cerium oxide (CeO_2) following photoexcitation using time-resolved spectroscopy combined with theoretical modeling. On femtosecond timescales, light absorption initiates rapid changes in the electronic structure, followed by lattice distortions. The research is supported by constrained density functional theory calculations explaining the charge distribution and structural changes in excited states. The results show how photoexcited materials evolve from an initially non-equilibrium electronic state toward a modified structural configuration, highlighting the role of photoinduced defect-like states in determining material behavior. These findings improve the understanding of light-driven processes in ceria and are relevant for its applications in photocatalysis, energy conversion, and oxide-based electronic devices.

Advanced Electronic Materials, DOI: 10.1002/aelm.202500429

Selective Tracking of Charge Carrier Dynamics in $CuInS_2$ Quantum Dots

The study combines ultrafast optical spectroscopy with femtosecond X-ray absorption spectroscopy at an X-ray free-electron laser to directly probe charge-carrier dynamics in $CuInS_2$ quantum dots. Photoexcited holes leave Cu atomic sites on sub-picosecond timescales, and no significant concentration of native Cu^{2+} defects was detected in Cu-deficient samples, suggesting that improved optical properties arise primarily from enhanced crystallinity and a reduced density of mid-gap trap states. Furthermore, Cu-deficient quantum dots exhibit greater resistance to photothermal damage under intense excitation conditions than Cu-rich materials. The research provides direct insight into the localization and transport of charge carriers in semiconductor quantum dots. These findings clarify the role of stoichiometry in determining the photophysical behavior of $CuInS_2$ nanomaterials and provide guidance for optimizing their optoelectronic performance.

ACS Nano, DOI: 10.1021/acsnano.4c18469

Capturing Ultrafast Spin Dynamics in Single-Molecule Magnets Using Femtosecond X-ray Emission Spectroscopy

Femtosecond X-ray emission spectroscopy (XES) together with ultrafast optical measurements are used to investigate photoinduced spin dynamics in manganese-based single-molecule magnets. Ultrafast structural distortions associated with the Jahn–Teller effect are identified. In the trinuclear Mn_3 complex, the X-ray probe provides unique sensitivity to the distribution of transient spin states populated within the first 100 fs after excitation. By combining complementary spectroscopic techniques with theoretical analysis, the authors disentangle the coupled electronic, spin, and structural dynamics that govern the excited-state behavior of these molecular magnetic systems. The results demonstrate the power of femtosecond X-ray spectroscopy for resolving elementary spin processes relevant to molecular magnetism and future quantum information applications.

The Journal of Physical Chemistry Letters, DOI: 10.1021/acs.jpclett.5c00383

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https://indico.solaris.edu.pl/event/31/

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- **HERCULES School 2027** – applications traditionally open in late August and close around **1 October 2026** for the 2027 edition.

Upcoming Conferences and Schools

- **SNIB2026 – German Conference on Research with Synchrotron Radiation, Neutrons, Ions and Accelerators at Large-Scale Facilities**
  📅 8–10 September 2026
  Hamburg, Germany
  Registration deadline: 3 August 2026.
- **Crosscarpatian Synchrotron School (CSS2026)**
  📅 Autumn 2026
  Kraków, Poland
  Thematic focus: X-ray spectroscopy and microscopy.

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We encourage PTPS members to share information about upcoming conferences, workshops, beamtime opportunities and training events for inclusion in future issues of the newsletter.

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