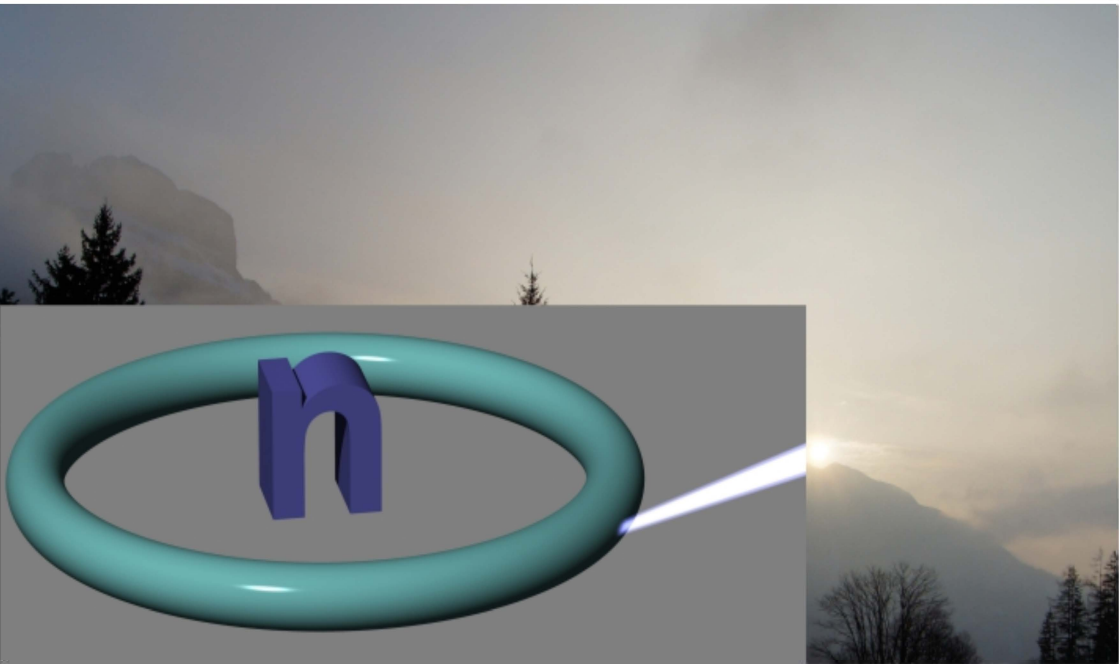
Bad Aussee (Austria), February 22nd-February 27th 2026

# The 13th European NESY Winterschool & Symposium on Neutron and Synchrotron Radiation

**Including topical highlight lectures on Big Data & Machine Learning and the 3rd CERIC Satellite Workshop, February 22nd**



# General

## Preface

The **NESY Winterschool & Symposium** is the traditional forum for Austrian neutron- and synchrotron radiation (NESY) users, with the aim to present and discuss new scientific achievements and to educate young academics in the field. The event was established in 1999 with the 1st *NESY Winterschool Planneralm* and was since then organised bi-annually until 2019. Due to the Covid pandemic induced interruption the event was shifted to the even-numbered years and now we are very happy to organise already the **13th European NESY Winterschool & Symposium 2026 on Neutron and Synchrotron Radiation**.

While in the first couple of years the event was "a School only", it developed into a mixed format of "School and Symposium". The tutorials in the morning cover modern neutron-, synchrotron- and free-electron laser sources as well as introductory lectures on a large variety of techniques employed by Austrian users at Europe's large scale research facilities. After a"skiing break" in the afternoon, the scientific part with *invited* and *contributed scientific talks* takes place. *Keynote lectures* related to the topical highlights of this year – Big Data and Machine Learning in neutron and synchrotron research. Finally, open-end *poster sessions* with drinks and discussions conclude the meeting days.

Prior to the NESY school & symposium, there will again be a complementary satellite event on Sunday -the **3rd CERIC workshop**- presenting activities of the European CERIC-ERIC consortium. CERIC-ERIC offers additionally to the NESY-techniques, complementary characterisation techniques that allow to receive a complete picture of the samples examined.

The topical focus of the NESY school & symposium was set to **Big Data & Machine Learning**. Experiments at large scale NESY facilities can particularly profit from the new developments in these fields, as typically large amounts of different data sets must be stored, organised and evaluated, ideally on-the-fly during the experiments. For handling large data sets from in-situ or operando experiments of complex systems and extracting relevant information *artificial intelligence* (AI) based tools are already widely used and will become much more exploited in future. The event will cover also another important aspect dealing with the curation of data following the FAIR-data principle. Details will be presented by experts coming from the scientific com-

munity, but also from industrial partners offering data analysis and storage solutions supported by AI. We are very glad that we could attract excellent scientists as keynote- and tutorial speakers from Austria, and also international experts from universities and large-scale research facilities, like CERIC, ELETTRA, ISIS and HZB-Hereon, as well as from companies. Besides the focus on big data & AI, a broad range of topics from biology, physics, chemistry and materials science up to fundamental quantum-physical topics will be covered as well.

All in all, we have **43 NESY contributions** - 15 tutorials, 3 keynote lectures, 5 invited talks, 9 contributed lectures, and 11 posters - which means that the dominant part of the roughly 65 participants contribute actively to the success of the event. Additionally, the 4 CERIC tutorials on Sunday afternoon are also open for all participants.

We acknowledge the sponsoring from the companies Anton Paar, DECTRIS Cloud and Rigaku. Thanks to these sponsoring contributions, not only support of the social activities (drinks at the poster session) is possible, but they generally help to keep the conference fees low. A special sponsoring from DECTRIS Cloud is dedicated for the two **Young Scientist Awards: -one for the best lecture and one for the best poster-** not only scientific prestige but also a dedicated monetary value.

We are very grateful to all tutorial, keynote and invited speakers for agreeing to come on their own costs, and to many others who have contributed in one or another way. We are most grateful to Nadine Aichberger for taking over a considerable part of the organisational issues. Special thanks go to Gerhard Popovski for the layout and assembly of this abstract booklet.

We are looking forward to an inspiring and enjoyable NESY Winterschool and Symposium 2026 in Bad Aussee.

Leoben, February 2026 Rainer T. Lechner & Oskar Paris

## Program

| Sunday, February 22nd | |
|---|---|
| 13:00-13:30 | **CERIC Opening: H. Amenitsch** |
| 13:30-14:30 | *CERIC Tutorial:* **Andrew Harrison**<br>Introduction to CERIC |
| 14:30-15:30 | *CERIC Tutorial:* **Corneliu Ghica -*online***<br>Introduction to TEM techniques |
| 15:30-16:00 | *CERIC Tutorial:* **Zdravko Siketic**<br>Introduction to Ion Beam techniques |
| 16:30-17:00 | Coffee & Tea with Snacks |
| 17:00-18:00 | *CERIC Tutorial:* **Aljosa Hafner (Elettra, IT)**<br>Data Processing Pipelines and AI for Synchrotron and FEL Experiments |
| 19:00-20:00 | Dinner |

| Monday, February 23rd | |
|---|---|
| **Morning Session (Chair: H. Abele)** | |
| 8:30-9:00 | **NESY Opening: R.T. Lechner** |
| 9:00-10:00 | *Tutorial:* **Andrew Harrison**<br>NESY Techniques @ CERIC |
| 10:00-11:00 | *Tutorial:* **Andrew Harrison**<br>Neutron Sources & Techniques |
| 11:00-11:30 | Coffee & Tea only |
| 11:30-12:30 | *Tutorial:* **Heinz Amenitsch**<br>Synchrotron/XFEL |
| 12:30-16:30 | Free Lunch & Afternoon Break |
| 16:30-17:00 | Coffee & Tea with Snacks |

| **Afternoon Session (Chair: R.T. Lechner)** | |
|---|---|
| 17:00-17:30 | *Invited Talk:* **Bridget Murphy (Uni. Kiel, GER)**<br>Making Scientific Data FAIR and AI ready |
| 17:30-18:30 | *Keynote Talk:* **Max Burian (DECTRIS, CH)**<br>From Terabytes to Trust: Reproducible, Cloud-Native Workflows for Big-Data Science |
| 18:30-19:00 | Spare time slot |
| 19:00-20:00 | Dinner |
| **Evening Session** | |
| 20:00- | **Poster Session** |

| **Tuesday, February 24th** | |
|---|---|
| **Morning Session (Chair: R. Resel)** | |
| 9:00-10:00 | *Tutorial:* **Oskar Paris (TU Leoben, AT)**<br>Introduction to small-angle scattering |
| 10:00-11:00 | *Tutorial:* **Markus Wallerberger (TU Wien, AT)**<br>Navigating the bias-variance trade-off in materials science |
| 11:00-11:30 | Coffee & Tea only |
| 11:30-12:30 | *Tutorial:* **Stefan Kovarik (KFU Graz, AT)**<br>GIXD and GISAXS for Surface and Interface Science: Concepts, Methods, and AI-Based Analysis |
| 12:30-16:30 | Free Lunch & Afternoon Break |
| 16:30-17:00 | Coffee & Tea with Snacks |

| Afternoon Session (Chair: S. Kovarik) | |
|---|---|
| 17:00-17:30 | *Invited Talk:* **Alexander Bronstein (ISTA, AT) - *online***<br>Machine learning in natural and life sciences and engineering -*tbc.* |
| 17:30-17:50 | *Contributed Talk:* **Anmol Androta (TU Graz, AT)**<br>Resonant scattering with grazing-incidence X-ray diffraction for determining absolute configuration |
| 17:50-18:10 | *Contributed Talk:* **Sanjay John (TU Graz, AT)**<br>Deracemization in 1,1'- Binaphthyl Thin Films Studied by Electronic Circular Dichroism |
| 18:10-18:30 | *Contributed Talk:* **Max Rauscher (TU Leoben, AT)**<br>Beyond Global Metrics in Capacitive Water Deionization: Position-Resolved Operando X-ray Transmission |
| 18:30-19:00 | Spare time slot |
| 19:00-20:00 | Dinner |
| **Evening Session (Chair: B. Murphy)** | |
| 20:00-21:00 | *Keynote Talk:* **Heiko Weber (FAU, GER)**<br>Introduction to FAIRmat data management |
| 21:00- | **Poster Session** |

| Wednesday, February 25th | |
|---|---|
| **Morning Session (Chair: H. Amenitsch)** | |
| 9:00-10:00 | *Tutorial:* **Mial Lewis & Sarah Foxley (ISIS, STFC, UKRI, UK)**<br>Introduction to Data Reduction using Mantid |
| 10:00-11:00 | *Tutorial:* **Markus Mezger (Univ. Wien, AT)**<br>Soft Matter Studied by Scattering Techniques |
| 11:00-11:30 | Coffee & Tea only |

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|---|---|
| 11:30-12:30 | *Tutorial:* **Josef Keckes (TU Leoben, AT)**<br>X-ray and Neutron Diffraction on Polycrystalline Materials |
| 12:30-16:30 | Free Lunch & Afternoon Break |
| 16:30-17:00 | Coffee & Tea with Snacks |
| **Afternoon Session (Chair: J. Keckes)** | |
| 17:00-17:30 | *Invited Talk:* **Georg Pabst (KFU Graz, AT)**<br>A Bottom-Up Approach to Uncover Structural and Elastic Features of Cell Membranes Using Synchrotron and Neutron Scattering |
| 17:30-17:50 | *Contributed Talk:* **Michael Meindlhumer (TU Leoben, AT)**<br>In situ nanoscale stress mapping resolves the fundamental limits to the J-Integral concept |
| 17:50-18:10 | *Contributed Talk:* **Kevin Kutlesa (TU Leoben, AT)**<br>Nanodiffraction Analysis of Nanocrystalline Thin Films on Complex Substrate Geometries |
| 18:10-18:30 | *Contributed Talk:* **Fabian Gasser (TU Graz, AT)**<br>About Different Approaches to the Lorentz Factor for X-Ray Diffraction |
| 18:30-19:00 | **Austrian User Input for SAXS@ELETTRA 2.0** |
| 19:00-20:00 | Dinner |
| **Evening Session** | |
| 20:00-20:30 | **SAXS@ELETTRA 2.0** |
| 20:30-21:30 | **NESY Meeting** |

| Thursday, February 26th | |
|---|---|
| **Morning Session (Chair: M. Mezger)** | |
| 9:00-10:00 | *Tutorial:* **Herwig Michor (TU Wien, AT)**<br>Tutorial on inelastic and quasi-elastic neutron scattering |
| 10:00-11:00 | *Tutorial:* **Mahdi Hajlaoui (JKU Wien, AT)**<br>ARPES Studies of the Electronic Structure of Topological, Ferroelectric, and Magnetic Semiconductors |
| 11:00-11:30 | Coffee & Tea only |
| 11:30-12:30 | *Tutorial:* **Giovanni Zamborlini (KFU Graz, AT)**<br>Coupling molecules with ferromagnets |
| 12:30-13:00 | Spare time slot |
| 12:00-16:30 | Free Lunch & Afternoon Break |
| 16:30-17:00 | Coffee & Tea with Snacks |
| **Afternoon Session (Chair: M. Müller)** | |
| 17:00-17:30 | *Invited Talk:* **Stephan Wollstadt (Rigaku, GER)**<br>AI powered analysis tools implemented in Smartlab II |
| 17:30-17:50 | *Contributed Talk:* **Olga Resel (TU Graz, AT)**<br>On-Surface Synthesis of Porphyrin-based Two-dimensional Metal-Organic Frameworks: Structural Assembly, Electronic Properties and Transmetallation |
| 17:50-18:10 | *Contributed Talk:* **Katherine A. Mazzio (TU Wien, AT)**<br>Probing Anion Redox by X-Ray Spectroscopies in Doped Ni–Mn Based Layered Oxides for Na-Ion Batteries |
| 18:10-18:30 | *Contributed Talk:* **Marek Gocnik (TU Leoben, AT)**<br>Influence of trace and tramp elements on the phase transformation behavior of low-carbon steel analyzed by in-situ high-energy X-ray diffraction |

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|---|---|
| 18:30-19:00 | *Invited Talk:* **Jürgen Klepp (Univ. Wien, AT)**<br>Test of a very cold neutron interferometer based on nanodiamond-polymer composite gratings |
| 19:00-20:00 | Dinner |
| **Evening Session (Chair: O. Paris)** | |
| 20:00-21:00 | *Keynote Talk:* **Martin Müller (HZB Hereon, GER)**<br>Data & Science @ GEMS |
| 21:00- | **Poster Session** |

| **Friday, February 27th** | |
|---|---|
| **Morning Session (Chair: H. Michor)** | |
| 9:00-10:00 | *Tutorial:* **Hartmut Abele (TU Wien, AT)**<br>The Quantum Bouncing Ball & Gravity Resonance Spectroscopy |
| 10:00-11:00 | *Tutorial:* **Christian Prehal (PLU Salzburg, AT)**<br>Neutron and Synchrotron operando techniques for energy materials |
| 11:00-11:30 | Coffee & Tea only |
| 11:30-12:30 | *Tutorial:* **Thomas Sheppard (TU Wien, AT)**<br>In situ / operando X-ray imaging of functional materials and devices at work |
| 12:30-13:00 | Prizes & Closing |

# Sunday

## Afternoon

CERIC Tutorial, 13:30-14:30

### Introduction to CERIC.

Andrew Harrison
CERIC-ERIC, IT

CERIC Tutorial, 14:30-15:30

### Introduction to TEM techniques.

Cornelia Ghica
National Institute of Materials Physics, RO

Online presentation, if possible!

CERIC Tutorial, 15:30-16:30

### Introduction to Ion Beam techniques.

Zdravko Siketic
Ruder Boskovic Institute, HR

CERIC Tutorial, 17:00-18:00

### Data Processing Pipelines and AI for Synchrotron and FEL Experiments

Aljosa Hafner, George Kourousias, Roberto Pugliese
Elettra Sincrotrone Trieste, Italy

The future of scientific data processing at the CERIC partner facility Elettra Sincrotrone Trieste is built around MAPI (Modular Adaptive Processing Infrastructure), a facility-developed framework deployed across multiple beamlines to enable scalable, modular, and reproducible scientific-computing workflows on heterogeneous computing resources. In parallel, the Elettra Scientific & Quantum Computing team (SciQC) is advancing local AI capabilities, including on-premise Large Language Models and intelligent agents, to augment user support, streamline

analysis, and integrate AI natively into the synchrotron and FEL computing ecosystem.

# Monday

## Morning

NESY/CERIC Tutorial, 09:00-10:00

### Neutron & Synchrotron Techniques @ CERIC.

Andrew Harrison

CERIC-ERIC, IT

NESY Tutorial, 10:00-11:00

### Neutron Sources & Techniques.

Andrew Harrison

CERIC-ERIC, IT

NESY Tutorial, 16:00-17:00

### Synchrotron Radiation - Instrumentation & Techniques

Heinz Amenitsch

Institute of Inorganic Chemistry, Graz University of Technology, Stremayergasse 9/V, Graz, Austria & Austrian SAXS beamline @ ELETTRA

This presentation should give an overview from the fundamental aspects of X-ray interaction and their application till the practical issues for the design of an X-ray experiment. The following topics will be covered:

- Short introduction to X-ray interaction with matter
- What can you learn from X-rays?
- How are X-rays produced?
- How does a synchrotron work?
- Beamline components and outline
- FEL's and other new sources
- How to design my own beamline?

## Afternoon

Invited talk, 17:00-17:30

### Making Scientific Data FAIR and AI ready

Bridget Murphy
Kiel University, Germany

In science our data is precious. To use and reuse data, great care must be taken during and after experiments to capture and store not only the data and experimental parameters, but also to record the experiment and analysis workflows. This information is also vital for machine learning analysis applications. Making scientific data FAIR – Findable, Accessible, Interoperable and Reusable is possible due to the increasing digitalisation in our society. In this talk I will introduce the basics of best practice and illustrate tools and applications for high-level, rapid data analysis and discuss the challenge of implementing research data management in real experimental conditions.
I will introduce the DAPHNE4NFDI consortium [1] which brings together users representing key scientific application domains with the large-scale research facilities in photon and neutron science in order to advance the state of data management in the community. Uniquely, DAPHNE4NFDI engages directly with the user community and the large-scale research infrastructure facilities to develop user-driven data solutions to advance science experiments. The main goal of DAPHNE4NFDI is to make data from these experiments "FAIR", thereby making scientific work more efficient and gaining more knowledge from the data. This presentation will give an overview of our activities and elaborate on our progress, showcasing progress in our X-ray reflectivity use-case. Here in addition to electronic laboratory notebooks and persistent sample identifiers, the use case has developed ML-based data analysis [2]. This includes "ML-readiness" of (meta)data, beamline integration, and a reference data collection for ML model training and validation.
References
[1] A. Barty et al., Zenodo, 2023, DAPHNE4NFDI - Consortium Proposal, https://doi.org/10.5281/zenodo.8040606
[2] L. Pithan, et al., J. Synchrotron Rad. 30 (2023) 1064.
This work was supported by the consortium DAPHNE4NFDI in the context of the work of the NFDI e.V. The consortium is funded by the DFG - project number 460248799.

Keynote talk, 17:30-18:30

## From Terabytes to Trust: Reproducible, Cloud-Native Workflows for Big-Data Science

Max Burian

DECTRIS Ltd, Taefernweg 1, 5405 Baden, Switzerland

Modern neutron and synchrotron experiments can generate terabytes per day; the limiting reagent is no longer photons, but trust: can you (or a reviewer) re-run the analysis six months later and get the same scientific claim? This talk dissects the most common reproducibility traps in data-intensive materials science: data fragmentation, untracked parameters, drifting software environments, and data copies that silently diverge. I will introduce novel concepts such as: object storage as an immutable data backbone; workflow-as-code for provenance and auditability; containerized environments for repeatable execution; and event-driven/serverless steps that automate data conversion, processing, scientific quality control, metadata extraction, provenance capture, and notifications - so scientists spend time on interpretation, not file plumbing. I will close with the tensions that will define the next decade of experimental research: data governance vs. velocity, privacy vs. openness, and cost (and carbon) vs. scientific benefit.

# Tuesday

## Morning

Tutorial, 9:00-10:00

### Introduction to small-angle scattering

Oskar Paris
Chair of Physics, Technical University of Leoben

Small-angle scattering (SAS) is a widely used method to study structures at the nanometer scale. It probes macroscopic sample volumes and provides typically average values of size, shape and volume fractions of nanoparticles, nanopores or other nanoscale density inhomogeneities. Both, neutrons and X-rays can be used with similar resolution, ranging typically from about 1nm to a few hundred nm. X-rays – in particular at synchrotron radiation sources – allow fast in-situ or operando detection of changes of such nanostructures, or they can be used to probe very small volumes by using X-ray micro- or nanobeams combined with scanning imaging. Neutrons are restricted in this respect due to the rather low flux. But they have unprecedented advantages for very light elements such as hydrogen or lithium, particularly because of the possibility of contrast variation using isotope replacement. This tutorial will give an overview of "classical" SAS concepts as well as new developments including some application examples, with particular emphasis on the complementarity between X-rays and neutrons.

Tutorial, 10:00-11:00

### Navigating the bias-variance tradeoff in materials science

Markus Wallerberger
Institute of Solid State Physics, TU Wien, Austria

In this introductory talk, I aim to give a broad overview over machine learning (ML) and related techniques as they have been applied to problems in materials science. The fundamental tradeoff between uncertainty and bias inherent to learning shall serve as our guide. It explains why large-scale general purpose models, while valuable, have had limited impact in physics, and why on the other hand simple ML models tailored to specific problems have led to breakthroughs in molecular dynamics and quantum field theories. Time permitting, we will

turn to physical interpretation and phase transitions in the the tradeoff itself.

Tutorial, 11:30-12:30

## GIXD and GISAXS for Surface and Interface Science: Concepts, Methods, and AI-Based Analysis

Stefan Kowarik

Institute of Chemistry, KFU Graz, Austria

Grazing-incidence X-ray diffraction (GIXD) and grazing-incidence small-angle X-ray scattering (GISAXS) are powerful techniques for probing the structural properties of surfaces, thin films, and buried interfaces. By exploiting shallow incidence angles, they provide enhanced surface sensitivity while retaining access to in-plane and out-of-plane structural information across multiple length scales. This lecture introduces the fundamental principles of GIXD and GISAXS, covering experimental geometries, contrast mechanisms, and characteristic data features. Applications in surface and interface science are discussed, including crystalline ordering, nanostructure morphology, and time-resolved in situ/in operando studies. The second part of the talk highlights how machine learning and generative AI approaches support data interpretation through pattern recognition and feature extraction, such as automated Bragg reflection detection, as well as structure solution workflows ranging from classification and structure matching to unit-cell determination for unknown materials and complex phase mixtures.

## Afternoon

Invited Talk, 17:00-17:30

### Machine learning in natural and life sciences and engineering -*tbc.*

Alexander Bronstein

IST Austria, AT

Online presentation, if possible!

Contributed Talk, 17:30-17:50

### Resonant scattering with grazing-incidence X-ray diffraction for determining absolute configuration

Anmol Andotra(1,2), (1) Fabian Gasser (2) Ferdinando Malagreca (3) Roland C. Fischer (2,4) Yves H. Geerts (1) Roland Resel

(1) Institute of Solid-State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria (2) Université Libre de Bruxelles (ULB), Faculté des Sciences, Laboratoire de Chimie des Polymères, CP 206/01, Boulevard du Triomphe, 1050 Bruxelles, Belgium (3) Institute of Inorganic Chemistry, Graz University of Technology, Stremayrgasse 9/V, A 8010 Graz, Austria (4) International Solvay Institutes of Physics and Chemistry, Université Libre de Bruxelles (ULB), CP 231, Boulevard du Triomphe, 1050 Bruxelles, Belgium

Chirality has become increasingly significant across a spectrum of disciplines, including chemistry, materials science, biology, and the pharmaceutical industry. Resonant (anomalous) X-ray scattering is a direct method for probing chirality in crystals. By tuning the incident energy near atomic absorption edges, resonant scattering breaks the symmetry between lattice planes (-h -k -l) and (h k l), known as Friedel's law, by introducing a measurable intensity difference between Friedel pairs. This principle has been well established in single-crystal diffraction for assigning absolute configuration using Bijvoet method. However, in many experimental geometries such as grazing-incidence X-ray diffraction (GIXD) access to complete Friedel pairs is restricted. This talk will describe recent efforts to extend resonant scattering into GIXD geometry, enabling the assignment of absolute configuration for the enantiomorphic chiral crystals of the Br-oxo molecule. Simulations of the energy-dependent structure factors for different reflections display distinct energy dependences for the two absolute configurations, whereas

others remain identical. By comparing the measured and simulated energy-dependent intensities, absolute configuration can be assigned even without access to Friedel pairs. This approach opens new opportunities for studying chiral crystals and offers potential extensions toward thin films.

Contributed Talk, 17:50-18:10

## Deracemization in 1,1'- Binaphthyl Thin Films Studied by Electronic Circular Dichroism

Sanjay John (1), Ann Maria James (1), Fabian Gasser(1), Tiberiu-Marius Gianga(2), Giuliano Siligardi(2), Bastian Daniel(3), Yves H Geerts(4), Roland Resel(1)

(1) Institute of Solid State Physics, Graz University Technology, Petersgasse 16, Graz 8010, Austria. (2) B23 Beamline, Diamond Light Source, Diamond House, Harwell Science & Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK. (3) Institute of Molecular Biosciences, Humboldtstraße 50/III, University of Graz, Graz 8010, Austria. (4) Laboratoire de Chimie des Polymères, Faculté des Sciences, Université Libre de Bruxelles (ULB), Boulevard du Triomphe, CP 206/01, Bruxelles 1050, Belgium.

1,1'-binaphthyl (BINAPH) is an axially chiral molecule that crystallizes in either a racemic phase, consisting of an equal number of both enantiomers in the unit cell or in a chiral phase where only one type of enantiomer is present. Thin film crystallization of BINAPH are strongly influenced by the presence of a solid substrate, where selective adsorption at the substrate–liquid interface promotes heterogeneous nucleation and complete chiral phase formation. This study further explores the deracemization of BINAPH through the influence of a chiral additive, 1,1'-bi-2-naphthol (BINOL). Structural characterization by Grazing Incidence XRD using synchrotron radiation confirms that thin films prepared by solution processing crystallize preferentially in the chiral phase of BINAPH. The extent of deracemization and enantioselectivity is further investigated using electronic circular dichroism (ECD). For the first time, the solid-state ECD spectra of BINAPH thin films are recorded using conventional ECD spectrometer and synchrotron-based Mueller Matrix Polarimetry (MMP). Since conventional ECD measurements cannot resolve intrinsic ECD from linear anisotropies such as linear dichroism and birefringence, spatially resolved Mueller matrix polarimetry is employed to accurately extract true solid-state ECD. MMP mapping on the thin film samples reveals

localized chiroptical responses within the BINAPH thin films, providing direct insight into enantioselective crystallization and spatially resolved chiral purity.

Contributed Talk, 18:10-18:30

## Beyond Global Metrics in Capacitive Water Deionization: Position-Resolved Operando X-ray Transmission

Max Rauscher (1)

(1)Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, Montanuniversität Leoben, 8700 Leoben, Austria

Current capacitive water desalination evaluation mostly relies on effluent- and electrochemistry based global metrics [1]. While they are important for the description and optimization of device performance, they unfortunately don't allow insight into the underlying mechanisms of local charge storage and transport. We present a new position-resolved, operando synchrotron X-ray transmission approach that quantifies local ion concentration changes within a working flow-by CDI cell [2]. Bulk electrolyte and electrodes are independently measured. Using 15 mM CsCl to maximize X-ray contrast, we probe three flow rates and two hierarchical carbon electrodes to map spatial and temporal ion redistribution from inlet to outlet of the cell. The method captures both, high-flow operation and a "quasi-static" limit within the same platform, enabling in situ determination of salt adsorption capacity and charge efficiency without relying solely on effluent analysis. We observe a pronounced dependence on flow rate, with decreasing local desalination capacity toward the outlet at slower flows, indicating replenishment limitations. Across all conditions, the better-performing material exhibits higher absolute uptake and charge efficiency, consistent with dominant counter-ion adsorption promoted by ultra-micropores that are ionophobic at no applied voltage. Spatial analysis reveals a position-dependent uptake strongly influenced by cell geometry [2]. This framework establishes a versatile platform that is readily extensible to energy-tuned X-ray contrast and complementary scanning X-ray modalities (such as SAXS or XRF) for multi-ion and pore-specific studies.

[1] S. Porada, R. Zhao, A. Van Der Wal, V. Presser, P.M. Biesheuvel, Review on the science and technology of water desalination by capacitive deionization, Prog. Mater. Sci. 58 (2013) 1388–1442. https://doi.org/10.1016/j.pmatsci.2013.03.005.

[2] M.V. Rauscher, R. Kohns, M. Seyffertitz, S. Stock, S. Haas, V. Presser, C. Prehal, N. Hüsing, O. Paris, Beyond global metrics in capacitive water deionization: Position-resolved ion concentration from operando X-ray transmission, Desalination 623 (2026) 119849. https://doi.org/10.1016/j.desal.2026.119849.

## Evening

Keynote talk, 20:00-21:00

### Introduction to FAIRmat data management -*tbc*

Heiko Weber

FAU Nürnberg Erlangen, Germany

*-tba*

# Wednesday

## Morning

Tutorial, 9:00-10:00

### Introduction to Data Reduction using Mantid

Mial Lewis, Sarah Foxley
ISIS, STFC, UKRI

The Mantid project is a cross-facility collaboration that provides computational tooling to support the processing of data gathered from Neutron scattering or Muon spectroscopy experiments. This talk will present the Mantid Workbench software application, a package that provides graphical user interfaces, scripting capabilities and automated workflows to aid data reduction. Key Mantid concepts and functionality will be introduced such as data loading, data structures (workspaces), algorithms, plotting, and fitting. A walkthrough of a typical data reduction workflow will be undertaken with real neutron scattering data (permission pending). An update will be provided regarding current and future development of Mantid.

Tutorial, 10:00-11:00

### Soft Matter Studied by Scattering Techniques

Markus Mezger
Universität Wien, Fakultätszentrum für Nanostrukturforschung

X-ray and neutron scattering techniques offer unique capabilities to study soft condensed matter. In this tutorial I will introduce experiments and data analysis ranging from short range order in complex liquids to liquid crystals. Beyond bulk studies, high brilliant synchrotron radiation allows to study fast dynamics and structures adjacent to interfaces and in nanoscale confinement.

Tutorial, 11:30-12:30

## X-ray and Neutron Diffraction on Polycrystalline Materials

Jozef Keckes

Montanuniversität Leoben

Polycrystalline materials exhibit pronounced intrinsic gradients in microstructure and strain, whose magnitude scales inversely with grain size and which decisively influence their functional properties. X-ray and neutron diffraction techniques, operating with beam sizes ranging from the centimetre down to the nanometre scale, are particularly well suited to resolve such gradients in a position-resolved manner deep within the material volume. In this contribution, a concise and highly simplified introduction to diffraction theory is first provided, with the specific aim of highlighting the types of information that can be extracted from diffraction data. Subsequently, scanning diffraction approaches are demonstrated using selected examples, including strain and microstructure mapping in thin films, steel tubes and surfaces, railway rails, and wood. Most of these examples originate from industrial collaborations. The experiments were carried out at large-scale research facilities in Grenoble (ESRF), Hamburg (PETRA III), Munich (FRM II), and Berlin (BESSY). Finally, the presented results demonstrate that diffraction is not only a powerful tool for analysing material structure, but also a key methodology for the knowledge-based design and optimisation of functional material properties.

## Afternoon

Invited Talk, 17:00-17:30

### A Bottom-Up Approach to Uncover Structural and Elastic Features of Cell Membranes Using Synchrotron and Neutron Scattering

Georg Pabst

University of Graz, Institute of Molecular Biology, Humboldtstr. 50, 8010 Graz

Plasma membranes, the boundaries of cells, are inherently asymmetric —each leaflet possesses a distinct lipid composition that drives essential physiological processes such as signaling, trafficking, and membrane remodeling. To investigate how this asymmetry influences membrane structure and mechanics, we create compositionally controlled, ≈100 nm asymmetric lipid vesicles, with the option to incorporate specific membrane proteins. By combining complementary SAXS and SANS techniques, we resolve leaflet-specific structures and contrasts. Notably, hydrogen/deuterium contrast variation in SANS allows us to isolate individual leaflet thicknesses and evaluate transleaflet coupling —how changes in one leaflet affect the other. Additionally, we determine the bending elasticities of these systems by analyzing their undulatory dynamics on the nanosecond timescale using NSE spectroscopy. This presentation will detail the experimental design, including contrast-matching strategies and the joint fitting of SAXS and SANS data, alongside key findings that highlight the unique ability of combining elastic and inelastic scattering to unravel unique properties of plasma membranes.

Contributed Talk, 17:30-17:50

### In situ nanoscale stress mapping resolves the fundamental limits to the J-Integral concept

Michael Meindlhumer (1), Juraj Todt (1), Anton Hohenwarter (1), Manfred Burghammer (2), Martin Rosenthal (2), Daniel Kiener (1), Jozef Keckes (1), Markus Alfreider (1)

Department Materials Science, Montanuniversität Leoben (1), ESRF - The European Synchrotron (2)

In order to interpret irreversible microstructural processes occurring during elastic-plastic fracture of nanocrystalline materials, it is vital to

elucidate multiaxial stress and strain fields in the vicinity of a progressing crack. Here, cross-sectional X-ray nanodiffraction with a spatial resolution of 200 nm was coupled with an in situ indentation device to uncover the multi-axial stress fields associated with crack growth in microcantilever specimens prepared from the nanocrystalline (nc) CoCrFeMnNi high-entropy alloy (HEA). Loads of 22, 45 and 34 mN with consecutively increasing displacement were applied, which correspond to conditions of elastic loading, crack tip blunting and void formation and coalescence, respectively. Exemplarily, at 45 mN, crack opening stresses increased to 4.5 GPa and up to 1 µm from the crack tip a distinct plastic zone formed governed by the elastic-plastic crack tip stress field. Further loading lead to a breakdown of the commonly assumed crack tip singularity and even lead to a significant decrease of the evaluated stress magnitude, suggesting strain softening within the nc HEA. Furthermore, stress data were used to evaluate the J- and/or K-values around the crack tip and cross-validate it with the sequential unloading approach. The quantitative experimental strain and stress results provide unprecedented insights into the gradual stress evolution at the crack tip and across the cantilever as well as associated fracture processes in nc materials.

Contributed Talk, 17:50-18:10

## Nanodiffraction Analysis of Nanocrystalline Thin Films on Complex Substrate Geometries

Kevin Kutlesa (1), Michael Meindlhumer (1), Juraj Todt (1), Peter Kunnas (1), Manfred Burghammer (2), Jozef Keckes (1)

(1) Montanuniversität Leoben, (2) European Synchrotron Radiation Facility Grenoble

Despite extensive optimization of thin film properties on planar substrates, the process-structure-property relationship on complex substrate geometries remains poorly understood due to characterization challenges. This contribution demonstrates the capability of synchrotron X-ray nanodiffraction to resolve nanoscale gradients in microstructure and residual stresses across thin films on non-planar geometries. First, the cutting edge area of a nanocrystalline $Al_{60}Ti_{40}N$ thin film, deposited by DC magnetron sputtering on a WC-Co cutting insert, was characterized by cross-sectional X-ray nanodiffraction (CSnanoXRD) at the ID13 beamline of the ESRF in Grenoble. A monochromatic X-ray beam was focused to a size of $75 \times 75$ nm$^2$ using Multilayer Laue lenses, enabling spatially-resolved scanning of a

$35 \times 35$ $\mu m^2$ region across the cutting edge. Next, a nanocrystalline multilayer thin film was analyzed within the same framework, resolving microstructural and residual stress gradients in 250 nm thin sublayers along the substrate edge. Up to 250.000 two-dimensional diffractograms were recorded with an EigerX 4M detector and evaluated with the pyFAI software package. Our results reveal that the functional properties of nanocrystalline thin films are substantially influenced by the substrate geometry. The CSnanoXRD characterization, corroborated by electron microscopy and micromechanical testing, provides insights for the application-oriented design of thin films within performance-critical regions.

Contributed Talk, 18:10-18:30

## About Different Approaches to the Lorentz Factor for X-Ray Diffraction

Fabian Gasser (1), Josef Simbrunner (2), Benedikt Schrode (3), Armin Moser (3), Nicola Demitri (4), Václav Holý (5), Roland Resel (1)

(1) Graz University of Technology, (2) Medical University Graz, (3) Anton Paar GmbH, (4) Elettra-Sincrotrone Trieste, (5) Charles University Prague

The quantitative evaluation of X-ray diffraction data requires the determination of reliable peak intensities. In this context, intensity correction factors play a crucial role, as they allow to directly relate measured peak intensities to squared structure factors. Among the correction factors, the exact knowledge of the Lorentz factor is particularly important. There are two approaches to evaluating the Lorentz factor. The first approach is based on the integration of the total diffracted intensities in reciprocal space coordinates, where the Lorentz factor represents the Jacobian determinant relating real-space integration variables to reciprocal-space coordinates. In the second approach, denoted as the velocity factor, the Lorentz factor is derived from the time required for a reciprocal lattice point to pass through the Ewald sphere during a diffraction experiment. In this work, it is shown that both models yield equivalent results for the Lorentz factor for the most widely used experimental techniques, including angle-dispersive powder diffraction, grazing-incidence diffraction, and single-crystal diffraction. By bringing the two approaches together, this work clarifies the physical meaning of the Lorentz factor and resolves apparent inconsistencies between different textbooks and research articles.

# Thursday

## Morning

Tutorial, 9:00-10:00

### Tutorial on inelastic and quasi-elastic neutron scattering

Herwig Michor
Institute of Solid State Physics, TU Wien, Austria

Inelastic neutron scatting (INS) is a fundamental microscopic technique to study the energy and momentum dependence of excitations related to lattice-, spin-, and orbital degrees of freedom in solids. Quasi-elastic neutron scattering (QENS) is a closely related form of INS applied to study excitations related to random interactions such as diffusive motion in liquids, biomolecular dynamics or paramagnetic spin-fluctuations. We will review the principles of INS and QENS, some basic instrumental setups and methods. As practical examples we briefly spotlight INS and QENS studies of some rare earth intermetallic compounds with respect to nuclear INS (e.g. phonon excitations) and magnetic INS and QENS related to crystalline electric field effects and paramagnetic fluctuations, respectively.

Tutorial, 10:00-11:00

## ARPES Studies of the Electronic Structure of Topological, Ferroelectric, and Magnetic Semiconductors

Mahdi Hajlaoui (1), Tetiana. Zakusylo (1), Gauthier. Krizman (2) Natalia. Olszowska (3), Jaime. Sánchez. Barriga (4), Ondřej. Caha (5), Juraj. Krempaský (6), Dominik. Kriegner (7), Libor. Šmejkal (7), Tomas. Jungwirth (7), Jan. Minar (8), and Gunther. Springholz (1)

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Angle-Resolved Photoemission Spectroscopy (ARPES) is a powerful experimental technique for directly probing the electronic band structure of solids, providing momentum- and energy-resolved information on occupied electronic states. In the context of semiconductors, ARPES offers unique insight into band dispersion, band gaps, surface and interface states, and many-body interactions, making it an essential tool for understanding both fundamental properties and the functional behavior of advanced materials. In this talk, we introduce the basic principles of ARPES, discussing how the photoemission process enables direct access to the electronic structure in reciprocal space. We highlight the main advantages of this technique, particularly in the UV photon energy range, where ARPES is especially well suited for studying surfaces and two-dimensional materials owing to its intrinsic surface sensitivity and high energy and momentum resolution. At the same time, we address the key limitations of ARPES for studying three-dimensional materials, and discuss how one can distinguish between surface and bulk states, as well as the constraints related to momentum conservation. To illustrate the capabilities of ARPES for semiconductor research, we present representative examples from three classes of materials studied

in our group. For topological materials, ARPES has played a crucial role in identifying topologically protected surface states and topological phase transitions [1]. In magnetic semiconductors, ARPES allows us to investigate the impact of magnetic order on the electronic band structure [2,3], providing, for example, evidence of the altermagnetic phase transition in alpha-MnTe. Finally, in ferroelectric and polar semiconductors, such as GePbTe (111), ARPES provides insight into Rashba-type spin splitting and the coupling between electronic structure and ferroelectric polarization [4,5].

[1] Rienks, E. D. L. et al. Nature 576, 423–428 (2019)
[2] Hajlaoui, M. et al. Adv. Mater. 2314076, 1–8 (2024)
[3] Krempaský, J. et al. Nature 626, 517–522 (2024)
[4] Krempaský, J. et al. Phys. Rev. B 94, 1–7 (2016)
[5] Krizman, G. et al. Adv. Mater. 36, 2310278 (2024)

Tutorial, 11:30-12:30

## Coupling molecules with ferromagnets

Giovanni Zamborlini

Institute of Physics, NAWI Graz, University of Graz, Austria

Molecule–substrate interactions play a crucial role in both spin and charge injection in organic-based devices, significantly impacting the overall physical, magnetic, and chemical properties of the interface. In this talk, I will illustrate some examples of how the molecule–substrate interaction alters the pristine properties of selected molecular complexes. In this regard, synchrotron radiation techniques provide fundamental tools to experimentally access electronic and structural properties at the atomic level. At first, I will describe how oxygen adsorption strongly modifies the electronic properties of pristine Fe surface (O-Fe), enhancing electron correlation[1]. The spin-dependent electronic structure can be accessed by spin-resolved photoemission electron microscopy measurements coupled with theoretical methods beyond including the effect of electron correlation. Then, via a combination of photoemission orbital tomography, scanning tunneling spectroscopy, and Hubbard-corrected DFT, the unexpectedly strong molecule-metal bonding between the pentacene molecule and O-Fe will be unraveled [2]. Finally, I will show how we can build a tunnel junction starting from the O–Fe substrate and pentacene, by separating them via a thin MgO layer [3]. The MgO barrier promotes double integer charge transfer populating the lowest unoccupied molecular orbital (LUMO) of pentacene with two electrons injected via tunneling from the underlying O-Fe substrate. Moreover, by tuning the work function (WF) of

the MgO film, we can control the LUMO energy over a wide range. Changing the growth conditions of the MgO film allows us to introduce an oxygen interlayer between MgO and Fe(100), which quenches the charge transfer at the interface [4].

[1] D. M. Janas et. al. Advanced Materials 35, 2205698 (2023).
[2] D. M. Janas et. al. under review in Small (2025).
[3] D. M. Janas et. al. In preparation (2025).
[4] D. M. Janas et. al. under review in Advanced Science (2025).

## Afternoon

Invited Talk, 17:00-17:30

### AI powered analysis tools implemented in SmartLab II

Stephan Wollstadt
Rigaku Europe SE

Artificial intelligence (AI) is increasingly transforming X-ray diffraction (XRD) data analysis. This presentation introduces AI-powered analysis tools implemented in *SmartLab Studio II* for powder and thin-film XRD. Deep-learning models based on Vision Transformer architectures enable robust, profile-based phase identification without peak search, significantly improving accuracy for complex materials with overlapping peaks or poor crystallinity. In addition, AI-driven component decomposition and X-ray reflectivity analysis enhance mixture evaluation and thin-film modeling. Together, these methods demonstrate how AI can substantially improve the reliability and efficiency of XRD data evaluation.

Contributed Talk, 17:30-17:50

## On-Surface Synthesis of Porphyrin-based Two-dimensional Metal-Organic Frameworks: Structural Assembly, Electronic Properties and Transmetallation

Olga Resel (1), Valentin Mischke (2), Alessandro Namar (3), Manuel Valvidares (4), Pierluigi Gargiani (4), Martin Sterrer (1), Mirko Cinchetti (2), Erik Vesselli (3), Giovanni Zamborlini (1,2)

(1) University of Graz, (2) TU Dortmund University, (3) University of Trieste, (4) ALBA Synchrotron Light Source

Metal-organic frameworks (MOFs) – porous, ordered and periodic structures consisting of metal atoms and organic linkers – are attracting significant interest due to their ability to host metal nodes that serve as active sites for molecular binding, catalysis and magnetic applications. Moreover, owing to the wide range of organic functional groups, MOFs can be designed with tailored electronic properties, even at the 2D level. Here, I will present a thorough characterization of a porphyrin-based 2D-MOF, obtained by cobalt coordination of self-assembled manganese tetrapyridyl porphyrin on Au(100). We assessed structural and electronic properties of this on-surface 2D-MOF via low energy electron diffraction, X-ray photoelectron and X-ray absorption spectroscopy. In particular, cobalt deposition leads to formation of a high-quality 2D-MOF atop Au(100), and, at the same time, promotes transmetallation at the porphyrin macrocycle (i.e. replacement of manganese with cobalt atoms), yielding a homometallic 2D-MOF with cobalt in two different oxidation states arising from non-equivalent coordination environments.

Contributed Talk, 17:50-18:10

## Probing Anion Redox by X-Ray Spectroscopies in Doped Ni–Mn Based Layered Oxides for Na-Ion Batteries

Katherine A. Mazzio

TU Wien

Understanding electrochemically driven structural and electronic transformations in battery electrode materials requires experimental probes that directly resolve element-specific redox processes and local bonding environments, capabilities uniquely enabled by synchrotron radiation. In current batteries, the positive electrode is the main bottleneck

for achieving high specific capacities, motivating new cathode materials. Traditional cathodes are layered transition-metal oxides that store charge via ion intercalation and transition-metal ("cation") redox. Additional capacity can be obtained by activating lattice oxygen redox at high potentials; however, oxygen redox is closely coupled to structural changes, voltage hysteresis, and long-term degradation. In this talk, I will present recent results on cation-doped Ni–Mn based layered oxides, illustrating how targeted doping modulates oxygen redox behavior and high-voltage stability.[1–3] Using operando and ex situ synchrotron diffraction and spectroscopy at multiple European large-scale facilities, we show how overlapping redox processes that are indistinguishable by electrochemistry alone can be disentangled spectroscopically. Resonant inelastic X-ray scattering (RIXS) is highlighted as a key technique enabling direct identification of distinct oxygen redox centers. Combined with transition-metal and dopant-specific X-ray absorption spectroscopy (XAS), these measurements reveal how dopants such as Mg modify metal–oxygen covalency and shift the energetic landscape of high-voltage reactions. By integrating RIXS, XAS, high-resolution X-ray diffraction (XRD), pair distribution function (PDF) analysis, and density functional theory (DFT), this work demonstrates how complementary synchrotron techniques provide mechanistic insight beyond electrochemical characterization alone.

References:

[1] Li, Y. et al. Adv. Mater. 2024, 36, 18, 2309842
[2] Li, Y. et al. Adv. Funct. Mater. 2025, e19132
[3] Li, Y. et al. preprint https://doi.org/10.21203/rs.3.rs-8109344/v1

Contributed Talk, 18:10-18:30

## Influence of trace and tramp elements on the phase transformation behavior of low-carbon steel analyzed by in-situ high-energy X-ray diffraction

Marek Gocnik (1), Lukas Hatzenbichler (1), Michael Meindlhumer (1,2), Phillip Haslberger (3), Matthew Galler (4), Andreas Stark (5), Claes-Olof A. Olsson (6), Jozef Keckes (1), Ronald Schnitzer (1)

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In the effort to decarbonize the steel industry, a new processing route combining scrap metal recycling with electric arc furnace (EAF) steelmaking is gaining prominence. This approach, while reducing carbon emissions, introduces trace and tramp elements that can significantly influence the phase composition and microstructure of the final steel products. Understanding these effects is crucial for optimizing material properties and ensuring performance consistency. In this study, the phase transformation behavior of low-carbon steel with varying concentrations of trace and tramp elements was thoroughly investigated. A reference alloy produced via the conventional blast furnace (BF) route was compared to two trial alloys processed through the EAF route with elevated levels of residual elements. To determine phase transformation temperatures and phase evolution during heat treatment, dilatometry experiments were performed alongside in-situ high-energy X-ray diffraction (HE-XRD). Rietveld refinement was utilized to quantify the volume fractions of ferrite, cementite, and austenite. Additionally, microstructural characterization was conducted using light optical microscopy (LOM) and scanning electron microscopy (SEM), including electron backscatter diffraction (EBSD). The EBSD analysis provided qualitative insights into the presence and distribution of martensite. The results indicate that the presence of trace and tramp elements broadens the critical transformation temperature range. Consequently, the formation of displacive phases, along with the retention of austenite, is promoted during cooling.

Invited Talk, 18:30-19:00

### Test of a very cold neutron interferometer based on nanodiamond-polymer composite gratings

Jürgen Klepp

Faculty of Physics, University of Vienna

Over the past decade, holographic nanodiamond–polymer composite gratings have been developed and optimized as efficient diffractive elements for very cold neutrons (VCN). We report on their characterization using light and their neutron-optical performance, including diffraction efficiency and angular selectivity for VCN at PF2 of the ILL. We explain their integration into a VCN interferometer. The layout of the interferometer and its implementation at the beamline are described. Preliminary measurements with VCN interferometer are presented. We discuss avenues for performance improvement and the way towards precision neutron phase measurements in the very cold regime.

## Evening

Keynote Talk, 20:00-21:00

### Data & Science @ GEMS

Martin Müller

Helmholtz-Zentrum Hereon, Germany

The Helmholtz-Zentrum Hereon develops and operates neutron and synchrotron radiation instrumentation for materials science investigations through its GEMS platform (`www.hereon.de/central_units/gems/about/index.php.en`) at the MLZ in Garching and at PETRA III in Hamburg. Operando diffraction and in particular time-resolved tomography experiments produce large amounts of scientific data. The talk will highlight some of the most demanding experimental techniques used at GEMS. In the effort to apply the FAIR principles to the GEMS data, Hereon works on the entire data pipeline at the levels of the research centre, of Helmholtz as well as at the national (DAPHNE4NFDI) and European (EOSC) level.

# Friday

## Morning

Tutorial, 9:00-10:00

### The Quantum Bouncing Ball & Gravity Resonance Spectroscopy

Hartmut Abele

Atominstitut – TU Wien, Stadionallee 2, 1020 Wien, Austria

We present a resonant spectroscopy technique devoted to the study of gravitation and the related cosmological problems of Dark Matter and Dark Energy. The object is a quantum mechanical wavepacket of an ultra-cold neutron, and the new method extends the techniques of Purcel, Rabi and Ramsey to neutron quantum states in the gravity potential of the Earth. The technique is named Gravity Resonance Spectroscopy (GRS) in close analogy to Magnetic Resonance Spectroscopy (MRS). Here a neutron in the gravity potential of the Earth is placed on a reflecting mirror, and transitions between the gravitational quantum states are performed by applying mechanical oscillations of the mirror with the proper transition frequency, whereas in MRS technique, an atom, a molecule or a nucleus with a magnetic moment is placed in an outer magnetic field and transitions between the magnetic Zeeman splitting are performed by applying proper oscillations of radiofrequency fields. Resonant transitions between several of the lowest quantum states are observed for the first time. The strength of GRS is that it does not rely on electromagnetic interactions. The use of neutrons as test particles bypasses the electromagnetic background induced by van der Waals forces and other polarizability effects providing the key to a sensitivity of several orders of magnitude below the sensitivity of atoms.

Tutorial, 10:00-11:00

### Neutron and Synchrotron operando techniques for energy materials

Christian Prehal

Department of Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Straße 2a, 5020 Salzburg, Austria

Operando neutron and Synchrotron techniques have emerged as pivotal in understanding complex chemical and physical processes in energy

storage, catalysis, and beyond. Attendees of this tutorial lecture will gain an overview of the working principles, advantages, and limitations of operando absorption spectroscopy, operando microscopy, operando tomography, and operando diffraction. Focusing on post-lithium-ion batteries, we explore operando small and wide-angle X-ray scattering (SAXS/WAXS) alongside small-angle neutron scattering (SANS) to unveil nanoscale electrochemical conversion during battery cycling. Specifically, I will demonstrate how operando SAXS and SANS, combined with machine-learning-assisted stochastic modeling and cryogenic electron microscopy allow quantification of the nanoscale phase evolution during the discharge and charge of Lithium-Sulfur batteries [1-3]. The research examples shown demonstrate how machine learning, together with complementary information from cryo-TEM, can extend the capabilities of structure-sensitive operando techniques such as neutron and X-ray scattering.

References:

[1] C. Prehal, V. Wood, et al. Nature Communications 2022, 13, 6326
[2] J.-M. von Mentlen, C. Prehal et al. ACS NANO 2025 19, 16626
[3] P. Dutta, C. Prehal, et al. ACS Energy Letters 2025, 10, 5722

Tutorial, 11:30-12:30

## In situ / operando X-ray imaging of functional materials and devices at work

Thomas Sheppard
TU Wien

Synchrotron radiation sources offer high intensity X-rays with ideal properties for imaging in 2D (microscopy) and 3D (tomography). The various contrast modes available to X-rays offer excellent flexibility and provide unique characterisation data which is unavailable to other analytical methods. When combined with in situ and operando methodology, this allows direct imaging of functional materials and devices at work. This contribution will outline the use of X-ray imaging to study structure-activity relations in functional materials, with a focus on heterogeneous catalysis. The principles of such measurements can however be applied to a broad range of sample systems.

# Poster

| Overview Poster | | |
|---|---|---|
| P-1 | Michael Haberl | Microsecond X-ray reflectometry |
| P-2 | Max Rauscher | Pore-Size-Dependent Ion Uptake in Capacitive Desalination via Operando SAXS on Carbons with Hierarchical Porosity |
| P-3 | Erwin Pfeiler | Toward Self-Driving Labs for X-ray Scattering with Bayesian AI |
| P-4 | Devina Gupta | Effect of Domain Sizes on The Long-Term Stability in Binary and Ternary Organic Solar Cells |
| P-5 | Claudia Obersnù | Seeding the vertical growth of laterally coherent coordination polymers on the rutile-$TiO_2$(110) surface |
| P-6 | Lorenz Gruber | Probing Storage Mechanisms in Biomass-Derived Hard Carbons for Sodium-Ion Batteries Using Operando SAXS |
| P-7 | Danny Milosavljevic | Inelastic neutron scattering study of the crystalline electric field in $DyNiC_2$ |
| P-8 | Josef Simbrunner | Finding crystal orientation in uniplanar textures |
| P-9 | Philipp Schwarz | In-situ Synchrotron SAXS/WAXS Study on the Aggregation of 1D CdSe-fibrils |
| P-10 | Johannes Liebhart | Structure–Function Relationships in Base-Functionalized MOFs investigated with SAXS and Gas Adsorption |
| P-11 | Rainer T. Lechner | ESUO - The European Synchrotron and FEL User Organisation: A brief introduction |

P-1

## Microsecond X-ray reflectometry

Michael Haberl (1), Maximilian Eder (1), Erwin Pfeiler (1), David Schumi-Mareček (1), Florian Bertram (2), Petr Mikulík (3), Stefan Kowarik (1)

(1) University of Graz, (2) Deutsches Elektronen-Synchrotron, (3) Masaryk University

We accelerate synchrotron X-ray reflectometry (XRR) by more than an order of magnitude and demonstrate the acquisition of full reflectivity curves within 213 $\mu s$ over a $q_z$ range of 0.05 - 0.35 $Å^{-1}$ at 0.001 $Å^{-1}$ resolution. This is achieved by rapidly sweeping the incidence angle with a high-speed galvanometer and recording the reflected beam on an area detector. The method preserves a monochromatic parallel-beam geometry, requires only straightforward geometric and exposure time corrections, and yields quantitative agreement with standard XRR in thickness, density, and roughness. At the shortest acquisition times, photon statistics enter the low-count Poisson regime, where conventional least-squares fitting becomes biased. We show that applying an Anscombe variance-stabilizing transform restores near-Gaussian error behavior and significantly improves fitting robustness, benefiting not only ultrafast XRR but reflectometry data in general at large $q_z$, where count rates are intrinsically low. This advance enables time-resolved studies of thin film growth, diffusion, photoswitching, and other rapid kinetic processes.

P-2

## Pore-Size-Dependent Ion Uptake in Capacitive Desalination via Operando SAXS on Carbons with Hierarchical Porosity

Max Rauscher (1), Richard Kohns (2,3), Johannes Liebhart (1), Malina Seyffertitz (4), Sylvio Haas (3,5), Oskar Paris (1)

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Global capacitive desalination metrics from effluent- and electrochemistry based data [1] are informative, yet they average over space and pore size. Consequently, they cannot resolve pore-size-dependent charging or ion transport, nor do they take ion gradients along the flow path into account. Building on our position-resolved operando X-ray transmission of capacitive desalination cells [2] we now pursue pore-size-resolved ion concentration dynamics within hierarchical carbon electrodes. Using operando small-angle X-ray scattering (SAXS) with aqueous CsCl, we leverage the high electron density of Cs to attribute scattering changes across different -regimes of the scattering vector magnitude (q) to micro-, meso-, and macropores. The model material—ordered mesoporous carbon with hexagonally arranged mesopores—leads to diffraction peaks in the small-angle regime, allowing mesopore filling to be distinguished from (disordered) micropore and macropore contributions appearing at higher and lower q -values, respectively. This work outlines a path to map local ion concentration in capacitive desalination not only along the flow direction, as shown previously [2], but also partitioned by the pore size class. In turn, we aim to reveal how pore hierarchy governs charge balancing, ion accessibility (including potential ionophobicity at zero voltage), and replenishment limitations under realistic operating conditions.

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Presser, C. Prehal, N. Hüsing, O. Paris, Beyond global metrics in capacitive water deionization: Position-resolved ion concentration from operando X-ray transmission, Desalination 623 (2026) 119849. https://doi.org/10.1016/j.desal.2026.119849.

P-3

## Toward Self-Driving Labs for X-ray Scattering with Bayesian AI

Erwin Pfeiler (1), Jan Schanbacher (1), Maciej Jankowski (2), Oleg Konovalov (2), Stefan Kowarik (1)

(1) University Graz, (2) ESRF Grenoble

We present a model-based Bayesian framework for self-driving scattering experiments that replaces fixed scan strategies and post-hoc analysis with real-time, uncertainty-aware decision-making. A physics-accurate forward scattering model is combined with a generative AI for posterior inference using normalizing flows, enabling continuous tracking of the full posterior distribution during data acquisition. Measurements are selected adaptively by maximizing information gain under realistic Poisson counting statistics. This closed-loop approach reduces acquisition time and beam damage while enhancing physical interpretability through real-time access to the full posterior. Although demonstrated using X-ray reflectometry (XRR), the framework is technique-agnostic and directly applicable to a broad class of scattering experiments with known forward models.

P-4

## Effect of Domain Sizes on The Long-Term Stability in Binary and Ternary Organic Solar Cells

Devina Gupta(1,2), Francesco D'Amico(3), Giovanni Birarda(3), Thomas Rath(2), Heinz Amenitsch(2)

(1) Central European Research Infrastructure Consortium, (2) Institute of Inorganic Chemistry,Graz University of Technology, (3) Elettra - Sincrotrone Trieste S.c.p.A.

Non-fullerene acceptor (NFA) based Organic solar cells (OSCs) have achieved record-high power conversion efficiencies of over 20%. However, their long-term stability remains a bottleneck in their large-scale

production. In this study, we investigate the morphology-stability-performance relationship of two Y-series NFAs, Y6 and Y-Pr, in OSC blends and devices, utilising PTQ10 as the electron-donating polymer. While the two NFAs have a similar chemical backbone, they show different morphological properties in blends. With the use of synchrotron and lab techniques such as GIWAXS, AFM, IR, and Raman spectroscopy, we track the morphological and chemical changes manifested in these OSC blends under different degradation conditions. The device performance is also tracked to correlate these findings with the morphology data. This work provides further insights into the influence of domain sizes and phase purity of the active layer on the long-term stability of OSCs under different environments.

P-5

## Seeding the vertical growth of laterally coherent coordination polymers on the rutile-$TiO_2$(110) surface

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The controlled fabrication of ordered molecular architectures with tailored functional properties at solid surfaces represents a key challenge for nanotechnology and device miniaturization. Although coordination polymers are efficiently obtained via conventional solution-based chemistry, their transfer onto substrates with the chemical, spatial, and geometrical homogeneity required for device integration remains challenging. Here, we adopt an in situ, vacuum-based, layer-by-layer self-assembly approach in which the anchoring sites are provided by ordered monolayers of metal(II)-tetraphenylporphyrins (M-TPP, M = Cu, Zn, Co) grown on the rutile $TiO_2$(110) surface. The metal center embedded in the porphyrinic macrocycle offers a well-defined coordination environment, enabling selective axial binding of a second-layer ligand. The affinity of the different metal ions toward axial coordination is investigated by subsequent deposition of symmetric dipyridyl-naphthalenediimide (DPNDI). Linear dichroism in NEXAFS spectroscopy reveals that DPNDI adopts a standing-up configuration on Zn- and Co-TPP as a result of nitrogen–metal axial coordination, whereas it lies flat on the substrate in the case of Cu-TPP. Calculations for a model pyridine ligand indicate stronger binding to Zn and Co centers, assisted by a surface trans effect, while the weaker

Cu–pyridine interaction is overcome by the strong DPNDI–$TiO_2$ interaction. The homeotropic alignment of the ditopic DPNDI ligand on Zn- and Co-TPP exposes coordination sites suitable for the growth of laterally coherent three-dimensional hetero-organic architectures.

P-6

## Probing Storage Mechanisms in Biomass-Derived Hard Carbons for Sodium-Ion Batteries Using Operando SAXS

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Sodium-ion batteries (SIBs) have gained significant interest as a sustainable and potentially low-cost energy storage technology [1], motivating intensive research into electrode materials and their structure-property relationships. Biomass-derived hard carbons (HCs) are commonly investigated as sustainable anode materials for SIBs [2], with their electrochemical performance being strongly governed by nanoscale structure. However, the exact sodium storage mechanisms in hard carbon and their impact on battery performance remain widely debated [3]. In this work, we demonstrate that resistive Joule heating of biomass precursors offers a rapid, low-cost, and tunable synthesis route, enabling systematic variation of carbonization conditions. Powder Small- and Wide-Angle X-ray Scattering (SAXS/WAXS), combined with analytical model-based data fitting, is employed to probe structural features across a broad range of length scales. The scattering analysis reveals temperature-dependent trends in structural parameters, with distinct responses observed for lignin- and cellulose-derived carbons. Operando SAXS measurements of HC anodes in SIBs provide time-resolved insight into sodium storage mechanisms, capturing concurrent structural contributions attributed to interlayer intercalation and pore filling during electrochemical cycling. Overall, this study highlights the effectiveness of Joule heating for producing biomass-derived HCs and demonstrates how advanced SAXS/WAXS analysis enables improved understanding of complex synthesis-structure-property relationships governing sodium storage in hard carbons.

P-7

## Inelastic neutron scattering study of the crystalline electric field in DyNiC2

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Rare-earth nickel dicarbides attracted attention, because of interesting properties such as superconductivity, magnetism, multiple charge density wave (CDW) transitions related to quasi-one-dimensional electronic features, and finally, a complex interplay of CDW order and rare earth magnetism. Here, we report on single crystal studies of thermodynamic bulk properties such as heat capacity and magnetic susceptibility of $DyNiC_2$ which are combined with powder inelastic neutron scattering studies conducted at the MAPS instrument at the ISIS neutron spallation source to analyse the crystalline electric field (CEF) splitting of the Kramers-type ($J = 15/2$) $4f^9$ state of $DyNiC_2$ in terms of a full CEF model. The latter is essential to further explore the peculiar quasi-quartet magnetic ground state of $DyNiC_2$ with two consecutive second order magnetic phase transitions, each releasing the entropy related to one CEF doublet state.

P-8

## Finding crystal orientation in uniplanar textures

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The crystallization of molecular materials on isotropic substrates typically results in a so-called fiber or uniplanar texture which comprises crystallites that share a common fiber axis perpendicular to the substrate surface, but which are azimuthally randomly oriented. The crystallographic characterization of such films is performed by grazing-incidence X-ray diffraction (GIXD). Two-dimensional reciprocal space maps are obtained, which incorporate the in-plane component qxy and the out-of-plane component qz for each diffraction peak. The exact

position of each diffraction peak depends on the crystallographic lattice and on the orientation of the unit cell relative to the substrate surface. The unit cell orientation can be characterized either by two rotation angles or by the Miller indices of the crystallographic plane parallel to the substrate surface. Equations are derived that allow the calculation of the orientation parameters and describe the relations between them. Dependent on the underlying unit cell, a manifoldness of possible orientations exists. Examples based on molecular crystals of pentacenequinone, diindenoperylene and binaphthalene are given which are illustrative examples comprising triclinic, monoclinic and tetragonal unit cells which have two, four and 16 possible crystal orientations, respectively.

P-9

## In-situ Synchrotron SAXS/WAXS Study on the Aggregation of 1D CdSe-fibrils

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Technical University of Leoben (1), Universtät Rostock (2)

In this work, we analyze a 1-dimensional, atomically defined, phosphonate-capped CdSe nanomaterial using in-situ SAXS/WAXS at the P62 beamline at DESY. The structure is related to the class of magic-size clusters that form in the early stages of nanocrystal synthesis. The material forms a colorless gel at room temperature and melts into individual fibrils that are stable up to 310 °C. The change in the aggregation state from bundles at room temperature to individual fibrils was studied in real time by SAXS/WAXS measurements. With this we could reveal the separation of the bundles above 60 °C and could follow the transformation to separated 1D fibrils with a diameter of only ∼2 nm and around 100 nm in length. During nanocrystal synthesis, they play a pivotal role in anisotropic growth of colloidal nanorods.

P-10

## Structure–Function Relationships in Base-Functionalized UiO-66: SAXS and Gas Adsorption Insights into Catalytic MOF Platforms

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Base-functionalized UiO-66 materials, modified with organic bases such as TBD, TMG, and DMAP, have been developed as versatile heterogeneous catalysts for thiol-ene covalent adaptable networks. This approach not only facilitates catalytic activity but also enhances the mechanical stability of dynamic polymer systems by improving stress relaxation control and minimizing creep. Our study focuses on the detailed structural characterization of UiO-66 and its base-functionalized derivatives. Using small-angle X-ray scattering (SAXS) and nitrogen physisorption techniques, we observed a significant decrease in BET surface area along with systematic changes in scattering profiles following base immobilization. Detailed analysis of peak positions and crystallinity reveals subtle but distinct differences within the framework between different functionalized samples. These structural modifications, caused by the organic base loading, give an insight for the catalytic perfomance.

P-11 (NESY)

# ESUO - The European Synchrotron and FEL User Organisation: A brief introduction

Rainer T. Lechner

Chair of Physics, Montanuniversitaet Leoben, Austria

The European Synchrotron and FEL User Organisation (ESUO) was founded in 2010 to represent all European photon science users. Today, ESUO represents about 30 000 users of the European synchrotron (SR) and Free-Electron Laser (FEL) facilities
Users from around 32 European & Middle East countries are represented by ESUO. The ESUO main goal can be seen in creating a truly European photon science community. ESUO's main objectives can be summarised in the following list:

- **Advocating** open access to European light sources
- **Forming** a pan-European light source user community.
- **Minimizing** administrative obstacles.
- **Increasing** competition to increase competitiveness.
- **Training** scientists hands-on.
- **Assisting** industry in innovation.

More details and current activities can be found on: `https://esuo.eu`

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*Abstract Book assembled by Gerhard Popovski & Rainer T. Lechner,*
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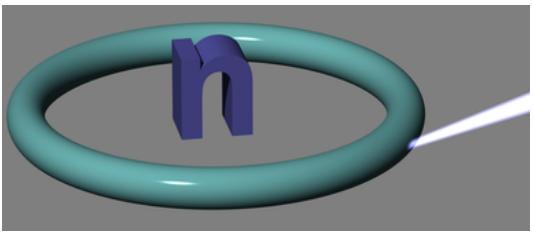

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