# Author: Prof. Bernd Rech Materials Challenges of Solar Energy Conversion and Storage: From a Photon Source Perspective Towards Next Generation Applications

Next generation solar cells, beyond lithium battery technologies, green hydrogen, sustainable fuels, and chemicals are essential building blocks for the future energy system. New materials are essential to enable breakthroughs in efficiency, stability, and scalability, as well as new approaches to close the carbon loop. To address these challenges, synchrotron sources have emerged as indispensable tools to identify and understand physical and chemical properties of materials, interfaces and devices for energy conversion and storage. The demand for operando investigations and advanced sample environments has strongly increased by our users, inhouse researchers and industrial partners. In this talk we will share latest results and experiences in photovoltaics, battery research and catalysis comprising highly efficient multijunction solar cells, operando studies on batteries and cooperation with industry on catalytic technologies, respectively.

# Author: Dr. Vera Steinmann Photovoltaics: from Lab to Scale How synchrotron experiments can accelerate materials development towards commercialization.

PV energy generation has grown at a historic pace, reaching 7% of global electricity generation in 2024. Yet, there is still room for growth. Especially low-cost PV could enable new green, lowcarbon markets. Perovskite-based thin-film PV holds tremendous promise to provide low-cost PV soon. High efficiencies have already been reported while materials and device stability are still inferior to state-of-the-art PV. X-ray microscopy can provide a unique lens to help accelerate learnings and stability improvements.

#### Author: Dr. Christopher Milne

# Probing ultrafast structural and electronic dynamics inadvanced materials using X-ray free electron lasers

#### European XFEL GmbH, Schenefeld, Germany 22869

X-ray spectroscopy and scattering allow a unique combination of electronic and structural information to be obtained from a variety of different types of samples in many different forms (solid, liquid, gas). The extension of these methods into the time domain has allowed measurement of dynamic processes, for example following charge transfer in molecular photocatalysts[1] or probing non-equilibrium melting in metals[2]. In recent years X-rays have started to become routinely used to measure light-activated processes using a pump-probe scheme, where the sample is photoexcited with light and then probed after a variable time delay using an X-ray pulse. With the recent development of X-ray free electron lasers (XFELs), time-resolved X-ray techniques have moved into the ultrafast regime, where the timescales of electron and nuclear motion can be accessed using the femtosecond X-ray pulses available from these facilities.

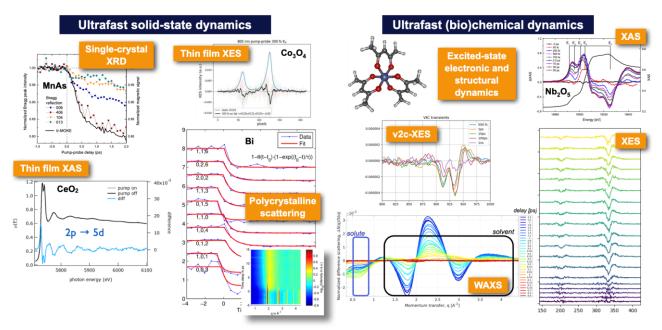


Fig. 1. Examples of the science and X-ray techniques performed at the FXE Instrument of the European XFEL

This talk will present an overview of how X-ray techniques are being used at XFELs to probe advanced materials and the type of information the measurements can provide[3]. The talk will introduce the European XFEL, a high-repetition rate XFEL facility located in northern Germany[4], and will show some examples of the types of measurements XFELs can perform and the scientific questions that can be answered using ultrafast X-ray techniques.

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3. Seddon, E. A. *et al.* Short-wavelength free-electron laser sources and science: a review\*. *Rep Prog Phys* **80**, 115901 (2017).

4. Tschentscher, T. *et al.* Photon Beam Transport and Scientific Instruments at the European XFEL. *Appl. Sci.* **7**, 592 (2017).

# Author: Dr. Jean-Luc Béchade

# Synchrotron source to analyse materials for nuclear applications, focus on zirconiumbased alloys fuel cladding of Pressurized Water Reactors.

Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, Gif Sur Yvette, 91191, France

The use of synchrotron radiation to study materials for nuclear applications is a widely used approach at CEA. It offers considerable advantages in terms of precision, resolution and diversity of analytical techniques. Synchrotron radiation, as an intense source of electromagnetic radiation, is particularly useful for exploring the structure, composition and behaviour of materials at the atomic and molecular scale, which is essential for materials used in nuclear applications.

These materials, subjected to extreme conditions such as high temperatures, high pressures and, of course, irradiation, undergo structural changes, chemical modifications and the appearance of defects and deformations at different scales (atomic to macroscopic). The techniques of X-ray diffraction, X-ray absorption spectroscopy and X-ray tomography, to name but the most common, are essential for synchrotron radiation, particularly *in situ* (in corrosive environments, at high temperatures or under stress, for example), if we are to gain access to the evolutionary kinetics of materials used in nuclear reactors.

This presentation will illustrate the contribution of synchrotron radiation by focusing on zirconium-based alloys fuel cladding containing uranium oxide fuel for pressurized water reactors (PWRs). Particular emphasis will be placed on the MARS beamline at the SOLEIL synchrotron facility, which can be used to analyse materials (solid or liquid) highly irradiated in reactors.

# Author: Myrtille O.J.Y. Hunault MARS beamline: a unique facility for the characterization of highly radioactive samples from the nuclear fuel cycle

Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP48, 91190 Gif-sur-Yvette, France The MARS beamline [1] at the SOLEIL synchrotron source belongs to the exclusive club of the few synchrotron beamlines dedicated to the investigation of highly radioactive materials using hard X-rays in the 3-35 keV energy range. Two experimental end-stations are available: i) a 4circle high-resolution diffractometer (allowing powder diffraction, surface analyses with combined texture and residual-stress analysis, reflectometry and reciprocal space mapping), and ii) a multimodal end-station for X-ray absorption spectroscopy techniques (XANES, EXAFS) as well as diffraction and scattering measurements (XRD and SAXS/WAXS) using a Pilatus 2M detector. Furthermore, a x-ray emission spectrometer enclosed in a He-filled chamber allows performing XES and RIXS measurements and the investigation of the low energy edges of actinides (M-edges) and other fission products with high energy resolution. [2] These techniques can be combined with imaging techniques based on X-ray microbeam raster scanning techniques or tomography reconstruction protocols.

Both end-stations are equipped with specific lead-shield to allow studying highly radioactive samples. Today, MARS is allowed to receive samples with radioisotope activities up to 2 Million times their isotope specific European exemption limits, and complies with all legal requirements and safety precautions to avoid contaminating aerosol dissemination and guarantee the public dose rate outside the beamline.

Thus the safety conditions offered on MARS allows using synchrotron techniques to directly characterize of the chemistry and microstructure of massive spent nuclear fuel [3] and high-level waste-glass samples. The applications of MARS beamline in the field of the nuclear fuel cycle are illustrated by selected highlights from recent or ongoing research.

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# Author: Prof. Rebecca Pittkowski Hydrogen and Beyond: Operando insights into electrocatalysts for Power-to-X

In Power-to-X applications, renewable electricity is converted into chemical energy carriers like hydrogen, ammonia, or synthetic fuels for energy storage and to decarbonize industrial applications. The re-conversion into electricity is possible either by fuel combustion or in fuel cells, which offer much higher efficiencies. Water electrolysis for hydrogen production is a key technology to enable PtX applications like eMethanol or sustainable aviation fuels (SAF). Different electrolyzer technologies (PEM, alkaline, and SOEC) are used to produce hydrogen, all with different prospects and limitations. Open research challenges include catalyst development focused on the limited use of critical raw materials (CRMs) without performance losses in terms of both activity and stability. Similarly, catalyst durability in hydrogen fuel cells with low Pt loadings remains an open challenge. Beyond hydrogen, electrocatalysis plays a major role in the sustainable production of fuels and chemicals, e.g., through CO<sub>2</sub> electroreduction. Fundamental insights into electrocatalyst activity, selectivity, and stability are possible with advanced structural characterization methods. Especially important are studies of operating catalysts and interfaces to determine real structure-property relations, as catalysts change their atomic structure and degrade. Time-resolved operando studies with high-energy X-rays under realistic conditions can, therefore, give insights into phase transitions, redox processes, and degradation mechanisms. By combining X-ray scattering techniques such as X-ray diffraction, small-angle Xray scattering (SAXS), and X-ray total scattering, complementary insight on different length scales of nanoparticle electrocatalysts can be obtained, and catalyst restructuring processes in the electrochemical environment can be followed.

# Author: Prof. Peter Wasserscheid<sup>1,2</sup>

# Chemical hydrogen storage - towards a hydrogen-free hydrogen economy

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Global logistics of renewable energy equivalents will create additional driving force towards a future hydrogen economy. However, the special nature of  $H_2$  requires dedicated infrastructures and this has prevented so far its massive introduction to the energy sector.

Recent scientific and technological progress in handling hydrogen in chemically bound form supports the technological vision that a future hydrogen economy may work without handling large amounts of elemental hydrogen using the existing infrastructure for fuels. Liquid Organic Hydrogen Carrier (LOHC) systems are composed of pairs of hydrogen-lean and hydrogen-rich organic compounds that store hydrogen by repeated, catalytic hydrogenation and dehydrogenation cycles.[1] CO<sub>2</sub>-based LOHC systems add interesting features to the more traditional systems based on aromatic/heteroaromatic compounds and their perhydro counterparts.[2]

The contribution will highlight fundamental and applied aspects of LOHC hydrogenation and dehydrogenation catalysis and the related processes. It will focus on the development of optimized catalytic materials for LOHC hydrogenation/dehydrogenation,[3,4] and on operational

stability aspects gained from demonstration units.[5,6] Application scenarios for stationary energy storage systems, hydrogen logistics and mobile applications will be discussed.

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# Author: MSc. John Bøgild Hansen

# Solid Oxide Cells in future sustainable energy scenarios: Opportunities and challenges.

Solid oxide cells are used both in electrolyzers (SOEC) and fuel cells (SOFC). They offer the highest efficiencies due to favorable thermodynamics and kinetics. In SOEC mode the system efficiency can be above 90 % and in SOFC mode above 60-65 %.

In electrolyzer mode they are especially well suited for integration with downstream synthesis of e-fuels like ammonia, methanol or Fischer Tropsch products because the waste heat from the syntheses can produce steam directly utilized as feedstock for the SOEC.

In fuel cell mode another feature is the capability to use a wide variety of fuels ranging from hydrogen to methanol, methane and ammonia in the latter cases benefitting from the ability to internally reform the fuel to hydrogen.

Several companies is presently ramping up manufacturing capacity, but challenges remain mainly related to performance degradations caused by a variety of chemical and physical processes more or less well understood, like segregation of nickel particles in the fuel electrode, poisoning by sulfur, silica, chromia etc. as well as thermomechanical problems.

# Author: Prof. Atsushi Urakawa

# Playing with thermodynamics and kinetics in $\text{CO}_2$ conversion catalysis

The amount of  $CO_2$  from the flue gas released by industrial processes and our activities is in the order of tens of gigatons globally. This enormous amount clearly points out that, besides actively demonstrated  $CO_2$  sequestration technologies, we need to urgently develop highly efficient  $CO_2$  conversion technologies to close the carbon cycle by recycling the carbon contained in  $CO_2$  into a usable form. One of the most promising paths to valorise a great amount of captured  $CO_2$  is its catalytic conversion to largely demanded chemicals like fuels. However, general challenges are its efficient activation and selective conversion to desired products. Numerous catalysts are developed to date; however, achieving high conversion efficiencies are often hindered by the high thermodynamic stability of  $CO_2$  as well as by the unfavoured reaction kinetics and thermodynamics.

In this talk, chemical and engineering strategies for efficient catalytic conversion of  $CO_2$  to chemical energy carriers are presented. Impacts of high-pressure conditions in combination with innovative catalysts on creating highly reactive environment as well as the importance of

*operando* studies will be presented for the synthesis of methanol, and CO among others. Furthermore, unique characteristics of unsteady-state operation to combine CO<sub>2</sub> capture and conversion in one process to produce syngas and methane are explained, highlighting the importance of *operando* methodologies to rationally develop and optimise catalytic materials and processes.

#### Author: Dr. Mateo Amatti Operando spatially resolved photoemission analysis of Fuel Cell components at the submicron scale.

Fuel cells are electrochemical devices providing efficient production of electricity directly converting the electrons exchanged in a redox reaction (such as a combustion) into electric current. One of the still unresolved issues that impedes their widespread applications is related to the limited durability of crucial components and mass transport events that deteriorate the performance.

Adding spatial resolution capabilities to synchrotron based X-ray spectroscopies, namely X-ray absorption spectroscopy, X-ray emission (fluorescence) spectroscopy, and X-ray photoelectron spectroscopy has opened unique opportunities for monitoring material changes and mass-transport events occurring at submicron length scales.

Recent achievements in the chemical and electronic characterization of fuel cells components performed at the Elettra synchrotron light source will be presented, in particular the work done with the two microscopes, the Scanning Transmission X-ray Microscope (STXM), hosted at the TwinMic Beamline [1], and the Scanning PhotoEmission Microscope (SPEM) hosted at the ESCA Microscopy beamline [2]. Both Microscope types use a direct approach to add the spatial resolution, i.e a submicrometric focused X-ray photon probe to illuminate the sample. The focusing of the X-ray beam is performed by Zone-Plates and the samples surface is mapped by scanning the sample across the focused beam.

In particular the talk will focus on experiments done in *Operando* to highlight the possibility to perform experiment in realistic conditions. For example, for SPEM, in the recent years the authors have developed photoemission imaging and spectro-microscopy methodology for a vast kind of possible sample environments for in-situ and operando electrochemistry experiments. Also, the so-called pressure gap, i.e. the lowest vacuum level admissible in operando studies, has been recently extended to near ambient values by using special cells [3]. [1] A. Gianoncelli et al. Journal of Synchrotron Radiation, 23(6), 1526-1537, 2016.

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# Author: Prof. Claire Villevieille TBD

# Author : Dr. Laura Simonelli FOSTERING BATTERY INNOVATIONS BY ADVANCED SYNCHROTRON TECHNIQUES: CHALLENGES AND OPPORTUNITIES ALBA Synchrotron Light Facility, Carrer de la Llum 2-26, 08290, Cerdanyola del Vallès, Spain

Over the years, synchrotron techniques are playing an increasingly important role in the development and innovations in battery science, due to their unique ability to provide accurate

information on the electronic structure of redox active elements, local and crystalline structure, and morphological information, also in operando conditions. Despite the potential innovative outcomes of synchrotron investigations, the generation of significant developments seems hindered by the resources needed to fully and quickly exploit these capabilities and the limited cooperation between academic and industrial parties.

Several challenges can be identified for the development of more performing and sustainable batteries. First of all, it has been widely demonstrated how in most of the cases it is needed a multi-modal and/or multi-scale approach, where only a combination of techniques is able to provide a comprehensive answer to the scientific question. On the other hand, massive data production due to such approaches and coupled to the operando capabilities imply challenges in the data analysis. Moreover, the variability of several reported results points out the need of developing well defined empirical strategies, including standardized data acquisition protocols and setups and automated recognition of artifacts, to correctly identify the correlations of interest and the right descriptors to evolve towards predictor approaches.

These challenges are addressed through examples, which highlights some necessary technical developments that are expected to foster battery innovation strengthening the cooperation between academics and industries to allow a faster outcome for the society.

#### Author: Dr. Marta Mirolo ReMade@ARI Project: how different networks join to boost Circular Economy

ReMade@ARI offers a platform of characterization techniques across Europe to accelerate the Circular Economy. The core of the project is the Smart Science Cluster (SSC), composed of Junior Scientists (JS) who are experts in the different analytical tools offered by the project. The JS support the users at different stages of the project: before the proposal submission, by suggesting the different techniques and helping with the proposal's writing; during the experiments, eventually travelling to the different facilities with the researchers and helping them with the experiments; and after the experiments, with the data analysis, whether possible. With the project nearing its conclusion, with only one call for proposals left (September 2025), some case studies will be presented, showcasing the support ReMade@ARI could provide. In particular, examples from the battery field and scattering techniques will be provided.

# Author: Dr. Jakub Drnec How Advanced X-ray Tools Unlock Energy Innovation and Help European Industry? Step out of your comfort zone.

The urgent need for energy innovation presents both a significant challenge and a opportunity for European industry. This presentation will demonstrate how moving beyond conventional research paradigms and embracing advanced X-ray tools is key to unlocking breakthroughs and maintaining a competitive edge. I will explore how stepping out of our scientific comfort zones to utilize the sophisticated capabilities of synchrotron light sources can directly translate fundamental insights into tangible industrial advancements, particularly in the energy sector. I will showcase concrete examples of this approach, drawing from applied research within the TEESMAT (Open Innovation Test Bed for Electrochemical Energy Storage Materials) project, which facilitates access for European companies to cutting-edge characterization of battery materials. These case studies will illustrate how advanced X-ray techniques like high-energy diffraction and scattering provide unparalleled *in situ* and *operando* understanding of material

behavior, essential for solving complex industrial problems and accelerating the development of next-generation energy technologies.

This talk serves as a call to action for both the scientific community and European industrial players. By fostering collaborations and daring to apply these powerful, often complex, X-ray methods, we can collectively push the boundaries of energy research, drive innovation, and secure a leading role for European industry in the global energy transition.

# Author: Dr Phil Cook Unlocking Industry Innovation with Big Science: Lessons from DTI's Partnerships at Synchrotrons and Neutron Facilities.

The Danish Technological Institute (DTI) is helping industry solve pressing materials and energy challenges by unlocking the capabilities of large-scale research infrastructures, such as synchrotrons and neutron sources. As a bridge between academia and industry, DTI's Big Science center leads collaborative research and development at both national and European levels. We are partners in numerous Horizon Europe projects including ReMade@ARI, InnoMatSyn, and ZEROSTEEL, and are coordinating the 9.2 M€ ACTNXT power-to-X project. This talk will highlight results from Innovation Fund Denmark projects on clean energy systems (HyFly, Low Cost H2) to illustrate the collaboration of technology infrastructures, research infrastructures, and industry. Drawing on experiences from the RITIFI project on industrial access, I will share concrete lessons and recommendations for making advanced facilities more accessible and impactful for industry, especially in the context of clean hydrogen development.

# Author: Dr. Robert Temperton Watching chemistry in-action using Soft X-ray Spectroscopy APXPS Group – MAX IV Laboratory

Soft X-ray spectroscopy provides a suite of powerful techniques for studying interfacial chemistry. Synchrotron techniques like X-ray Absorption Spectroscopy (XAS), X-ray Photoelectron Spectroscopy (XPS) and Resonant Inelastic X-ray Scattering (RIXS) are diversifying from the scientific playground of fundamental chemical physics research to the huge plethora of applied materials relevant to the energy sector. Developments in recent years are allowing this suite of spectroscopic probes, which were traditionally applied to post mortem analysis of samples, to study functional systems under operando conditions. Specifically, the HIPPIE beamline at MAX IV Laboratory, the worlds first 4<sup>th</sup> generation synchrotron facility, has focused on demonstrating what is possible at a modern, high-brilliance, soft X-ray beamline. Through the topics of batteries, thermal-catalysis and electro-catalysis, this talk with explore current trends and hypothesise on the direction of travel for how state-of-the-art soft X-ray spectroscopy facilities can be applied to energy materials research.

#### Author: Prof. Tejs Vegge

Accelerating materials discovery by machine learning and autonomous workflows for federated data generation and analysis – A case study for batteries and electrocatalysts

# Pioneer Center for Accelerating P2X Materials Discovery, CAPeX Technical University of Denmark, DTU Energy, 2800 Kgs. Lyngby, Denmark

The development of a framework for autonomous discovery plays a critical role in accelerating the discovery process for new sustainable and scalable battery materials and electrocatalysts. A central element in this process is the development of a federated closed-loop materials acceleration platform (MAP) infrastructure [1], where multiple and geographically distributed laboratories, large-scale facilities and computer/AI models can work jointly using autonomous workflows to co-optimize materials and device level properties [2]. A second critical component is establishing spatio-temporal structure-property relations of the dynamic processes at solidliquid interfaces, which is key to developing electrochemical conversion, e.g., Power-to-X and battery materials. Fundamental and performance-limiting interfacial processes like forming the Solid-Electrolyte Interphase (SEI) span numerous time- and length scales, and despite decades of research, the fundamental understanding of the structure-property relations remains elusive. Ab initio molecular dynamics (AIMD) generally provides sufficient accuracy to describe chemical reactions at these interfaces and can provide valuable complementary insights to complement experimental operando characterization techniques [3]. The cost is, however, prohibitively high to reach sufficiently long time- and length scales to ensure proper statistical sampling, and machine learning (ML) potentials offer a potential solution to this challenge, but training MLbased potentials capable of handling activated processes in organic or aqueous electrolytes remains a fundamental challenge since the potential must capture both intra- and intermolecular interactions in the electrolyte and during chemical reactions at the interface [4]. Here, we present new approaches using foundation models [5] and new transition state training sets [6] for chemical reaction networks and machine/deep learning models to predict the spatio-temporal evolution of electrochemical interphases. We also discuss the development of active learning methods to accelerate the segmentation of microstructures in non-destructive 3D imaging techniques, such as X-ray nano-holo-tomography, and enable the visualization of battery electrodes [7]. Finally, we discuss how such models trained on multi-sourced and multi-fidelity data from multiscale computer simulations, operando characterization, high-throughput synthesis, and testing to provide uncertainty-aware and explainable ML for early prediction of patterns from chemical spectra (Figure 1) [8], and how simple material representations like chemical formula without any structural information can sometimes achieve competitive property prediction performance beyond what our physics-based intuition would suggest given that such representations are 'incomplete' [9].

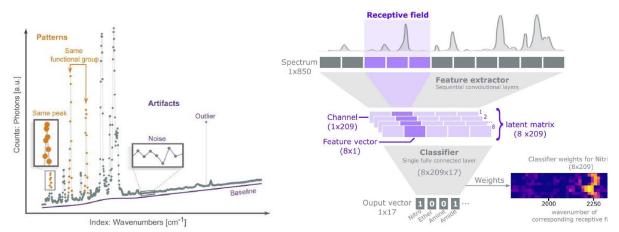


Figure 1: Understanding the patterns that neural networks can learn from chemical spectra [8].

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# Author: Prof. Helge Sören Stein Easy optimization, hard discovery, and how to engineer science

As the world moves towards electrification and emission-free processes, the demand for discovering and scaling new materials and processes for energy storage and conversion is greater than ever. Conventional research approaches struggle to keep pace with this need, necessitating a fundamental shift in how we conduct scientific discovery and optimization. In this talk, I will demonstrate how we can optimize formation processes and use them as a template for redesigning energy storage systems from the ground up. This approach not only accelerates performance improvements but also reveals new opportunities for breakthrough discoveries in battery and catalyst research. Our work at the Technical University of Munich (TUM) integrates data science, robotics, and chemistry to transform research. By leveraging machine learning, autonomous robotics, and automated high-throughput systems, we optimize not just individual materials but entire energy storage and conversion systems. Our research spans high-throughput coating, cell building, electrolyte formulation, and analysis, as well as parallel chemical reactors for catalyst optimization and building the infrastructure for automation, orchestration, and interpretation. To address these challenges, we employ Materials Acceleration Platforms (MAPs)—a fusion of combinatorial synthesis, highthroughput characterization, lab automation, and machine learning. MAPs facilitate both horizontal integration, by unifying experimentation, simulation, and data analytics, and vertical integration, by linking material design to device applications. This approach accelerates not only the research process itself but also its scalability and industrial implementation. A key example of our work is the FINALES framework, which enables decentralized control over distributed experiments across Europe, allowing us to optimize electrolyte formulations and predict device performance more effectively. In parallel, the HELAO framework provides real-time lab automation and data lineage management, ensuring rapid iteration and reproducibility in materials research. This talk will highlight the challenges and opportunities in optimizing virtually everything while unveiling how intelligent research design can turn seemingly intractable discovery problems into structured optimization tasks.

# Author: Dr. Bernd Hinrichsen

# Radically better materials characterisation: transforming research through synchrotron power.

The urgent global challenges of sustainable energy, climate change, and resource scarcity demand revolutionary materials solutions—solutions that can only emerge through transformative characterisation methods. While powder diffraction techniques pioneered by Debye, Scherrer, and Hull in 1916/17 established the foundation for atomic-level materials analysis, today's synchrotron-enabled methods represent a leap in materials science capability [1]

Synchrotron radiation sources, delivering brilliance up to 12 orders of magnitude higher than conventional laboratory instruments, have fundamentally altered our ability to interrogate materials across multiple length scales. This extraordinary power enables the detection and characterisation of trace phases below 0.1%, while providing unprecedented insight into defect structures, lattice strain, and atomic displacement parameters—critical factors governing material performance [2]

Most significantly, synchrotron powder diffraction enables systematic parameter space mapping—the comprehensive exploration of composition-structure-property relationships through high-throughput experimentation paired with sophisticated data analytics [3,4] This paradigm shift moves materials development beyond traditional trial-and-error approaches toward rational design based on fundamental understanding, with machine learning accelerating the discovery of structure-property correlations that would otherwise remain hidden.

Despite these transformative capabilities, synchrotron-based powder diffraction has remained largely inaccessible to many researchers. Momentum Transfer is changing this reality by democratising access to these powerful techniques, enabling researchers across disciplines to harness synchrotron capabilities for their materials challenges without requiring specialised expertise or privileged institutional access.

Join us to explore how synchrotron powder diffraction is revolutionising materials characterisation, accelerating discovery cycles, and making the once-elusive goal of "property by design" an achievable reality for addressing our most pressing technological challenges. References

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#### Dr. Justus Just

# Accelerating Insights into Complex Material Formation and Transformation Processes: Multimodal High-Throughput Schemes for In-Situ and Operando X-ray Experiments

Materials used for energy conversion or storage, such as in solar cells, batteries, and catalysts, are becoming increasingly complex and contain a multitude of elements. The specific properties of these materials, especially their energy conversion efficiencies, result from the complex interplay between precursors, intermediates, spectators, and products during synthesis processes. Knowledge-based discovery and tuning of these processes requires a fundamental understanding of their systematics, pathways, and kinetics. Due to the complexity of synthesis interactions, a multitude of experiments with a wide variation of parameters investigated from complementary perspectives is required.

Recent developments in synchrotron and beamline instrumentation across many facilities enable combined in situ experiments with complementary techniques to be performed simultaneously, i.e., multimodal experiments, with time resolutions in the millisecond to second range. These experiments provide unprecedented insight into formation and transformation processes by combining complementary perspectives. However, understanding correlations in complex processes often requires systematically investigating a multitude of process parameter variations, which can be tedious and time-consuming in manual experiments. Transitioning to robotic and high-throughput schemes for this type of complicated in situ/operando experiment removes current bottlenecks and enables the investigation of wide parameter spaces, facilitating a fundamental understanding of complex formation and transformation processes.

This talk will explore methodologies and capabilities for high-throughput schemes applied to in situ and operando experiments in the fields of batteries, catalysis, and photovoltaics. Recent developments at the Balder beamline at MAX IV, which integrate robotic, high-throughput solution processing with in situ multimodal process analysis to explore the synthesis landscape of hybrid perovskite semiconductors, will be highlighted.

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# From X-ray nanoscopy to responsible use of resources in photovoltaics.

X-ray microscopy is indispensable for metrology in R&D of semiconductor devices. We will first set the stage of state-of-the-art X-ray imaging for semiconductor applications and make second the link to spatially resolved performance measurements through X-ray beam induced current (XBIC) and X-ray excited optical luminescence (XEOL). We will then showcase some applications exploiting the full suite of scanning X-ray nanoscopy for research of thin-film solar cells with absorbers made of Cu(In,Ga)Se2, CdTe, and metal-halide perovskites. Compared to the workhorse silicon, such thin-film absorbers require less energy in solar-cell production resulting in a shorter energy pay-back time. Devil's advocate may ask: who cares about the energy back-back time and availability of resources? And which role play storage rings in the landscape of photovoltaics?