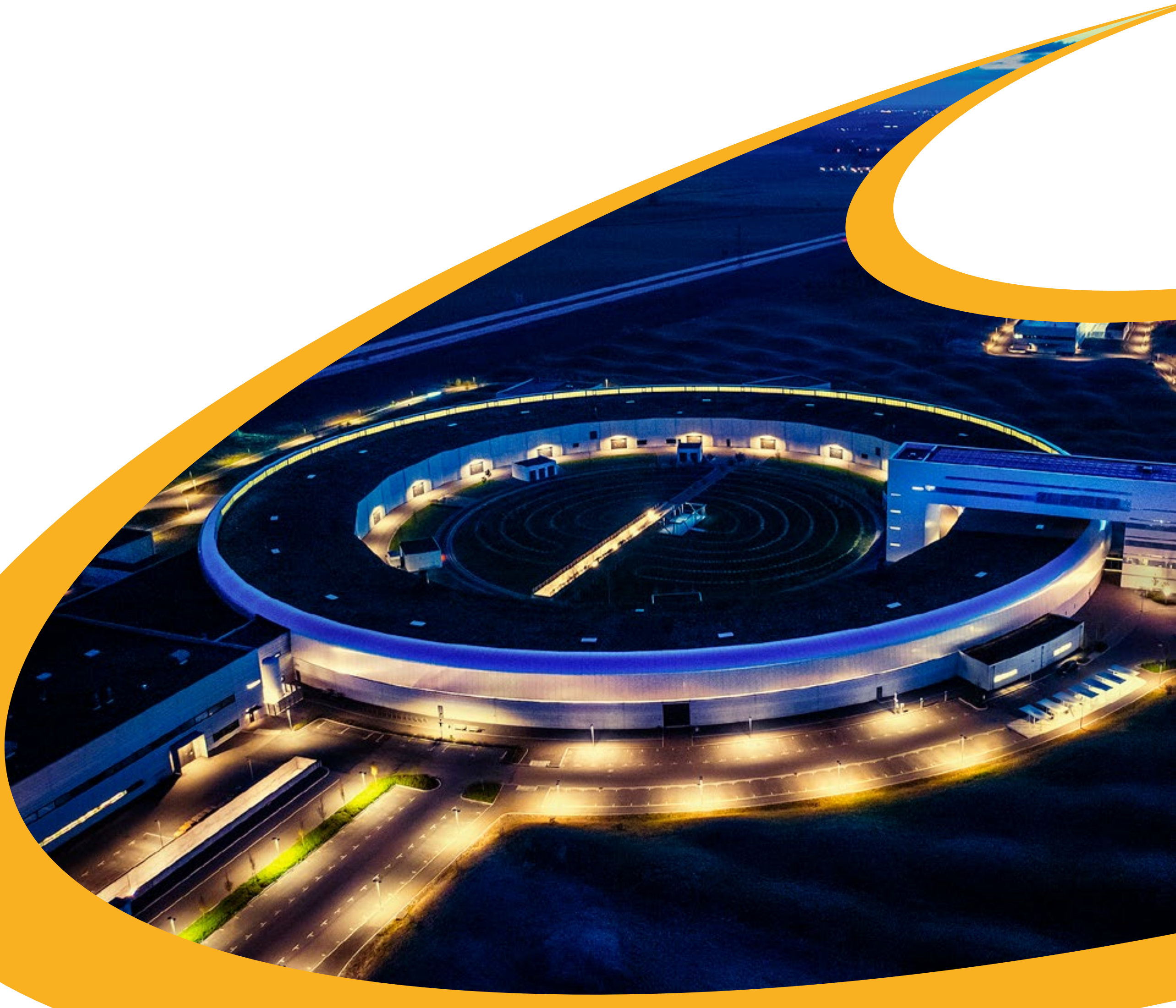
HIGHLIGHTS 2021



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if not otherwise stated, Kenneth Ruona, Johan Persson, Emelie Hilner

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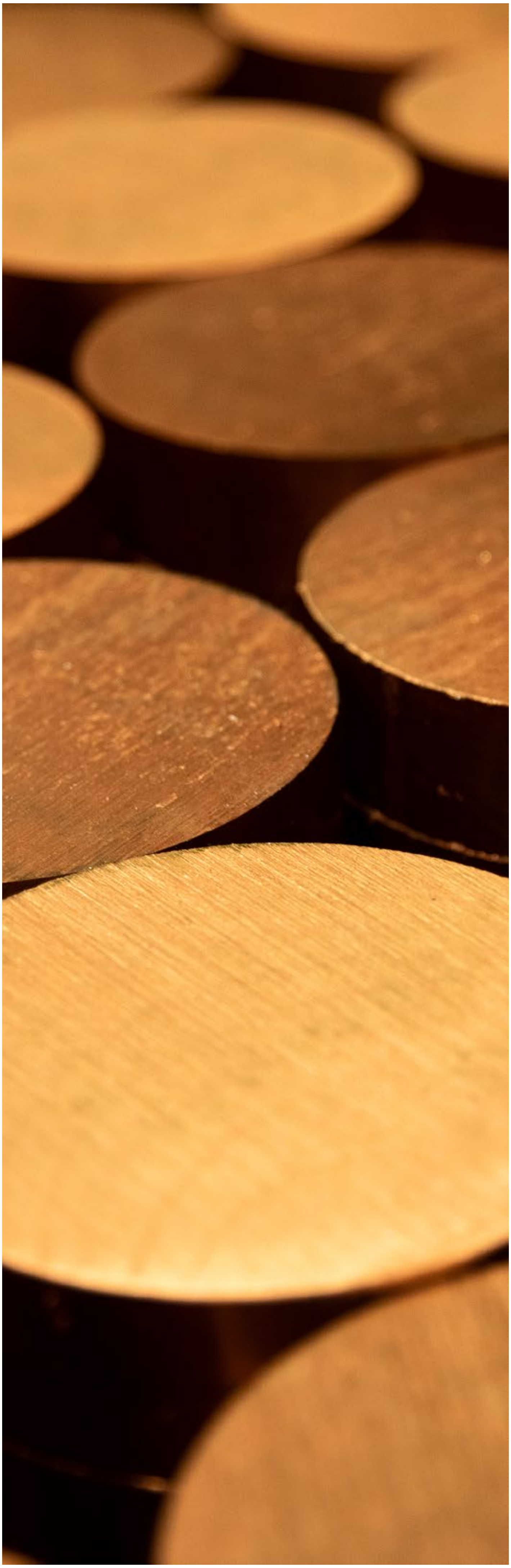


Foreword

MAX IV, like most lightsources around the world, continued to be affected by the COVID-19 pandemic throughout 2021. Our User Programme was impacted, as well as ongoing work at several beamlines, accelerator development and construction projects. However, some of our beamlines took the opportunity to ramp up construction activities. This was especially the case for our DanMAX, CoSAXS, and SoftiMAX beamlines, which welcomed their first user groups by the end of the year while continuously augmenting their experimental capabilities. These three beamlines offer modern X-ray capabilities for the research needs of the materials and chemical sciences, soft matter, and life and environmental sciences communities.

Other beamlines continued flourishing, as exemplified by the development of a second branch at HIPPIE. The new branch will be dedicated to studying the formation and breakthrough of the passivation layer on novel multicomponent alloys and chemical processes occurring at the electrode-electrolyte interfaces during the charging and discharging of Li-ion batteries. Also, an upgrade of the repetition rate of our linac to 10 Hz allowed a five-fold increase in the data acquisition time of experiments with short X-ray pulses offered by FemtoMAX.

The laboratory entered a warm shutdown during the first three months of 2021, and user site access was precluded most of the year. Still, our User Programme gradually restarted in the spring with reduced operations of the facility, for example, by offering the possibilities of mail-in and remote experiments for those experiments and beamlines that could accommodate such options. Our staff performed these experiments as no users were permitted onsite. BioMAX, our high-throughput macromolecular crystallography beamline designed to excel at supporting remote and mail-in experiments, continued to serve its user community throughout most of the year. By November, the laboratory resumed its usual User Programme, even though travel restrictions across the world sometimes impacted some experiments.

Despite the pandemic-related challenges and thanks to the many efforts of our staff and the excellent performance of our accelerators, 2021 was a year of delivering science from our academic and industrial user communities, as presented in these 2021 Highlights.

We hope you will enjoy the exciting examples in many diverse science areas such as the properties of advanced materials for the advancement of electronics, glacial rocks and Martian atmospheric chemistry, catalysis, development and instrumentation for our state-of-the-art beamlines, multimodal imaging for Alzheimer's research, solar cells and green future energy, a potential inhibitor for SARS-CoV-2, and signalling in plants.

The scientific productivity of MAX IV Laboratory continues to increase as more beamlines become available to the user community. Our publication database indicates that 138 peer-reviewed articles were published by staff and users in 2021, a 34% increase from 2020. More than one-third have an impact factor larger than their average of 7.1. We also celebrated the completion of 10 PhDs or MSc thesis using results from our beamlines.

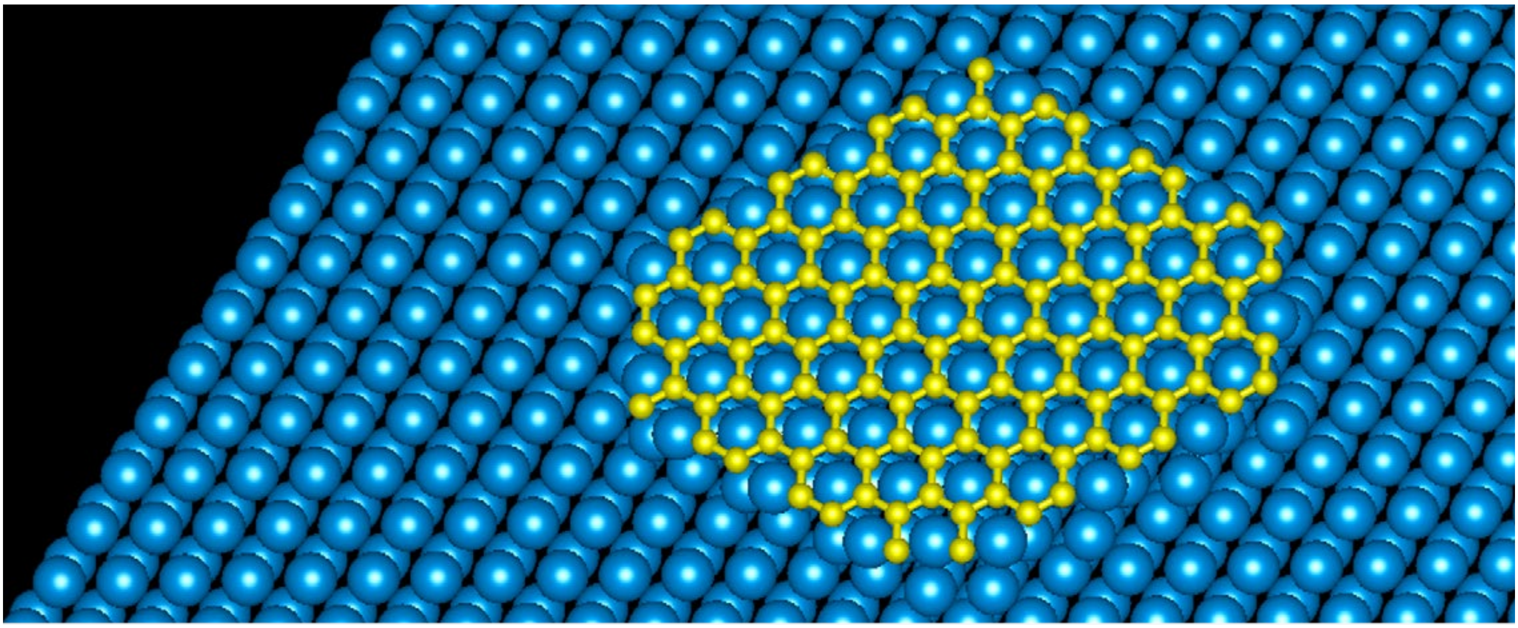
In October 2021, we held our 33rd MAX IV User Meeting as a hybrid event themed 'MAX IV in Focus.' This was also the time for one of us, Aymeric, to join MAX IV as Scientific Director for Physical Sciences.

Overall, we are pleased to see more beamlines contributing to more science. We also continue noting the solid regional position of MAX IV as a leading X-ray user facility serving a user community centrally located in northern Europe. In 2021, 79% of our users were affiliated with institutions in the north of Europe, but most notably in the Nordic (75%) and Scandinavian (71%) regions.

Once again, we are very grateful for the dedication, motivation, and engagement of our staff and user communities for continuing to deliver and contribute to a compelling science programme. A special thank you to all the contributors to our Science Highlights. We hope you will enjoy reading our 2021 Highlights and that it will continue inspiring you to use MAX IV to contribute to solving your research needs.

Marjolein Thunnissen & Aymeric Robert
Scientific Directors

Science Highlights



ADVANCED MATERIALS

Experimenting with borophene allotropes: honeycomb boron on aluminum

Scientists from Hokkaido University, St. Petersburg State University, and MAX IV's FlexPES examined whether honeycomb boron can function as a structural analogue 2D material to graphene. Core-level X-ray spectroscopies, scanning tunneling microscopy, and Density Functional Theory calculations were used to analyse the structure and electronic properties of honeycomb boron's reaction with aluminum.

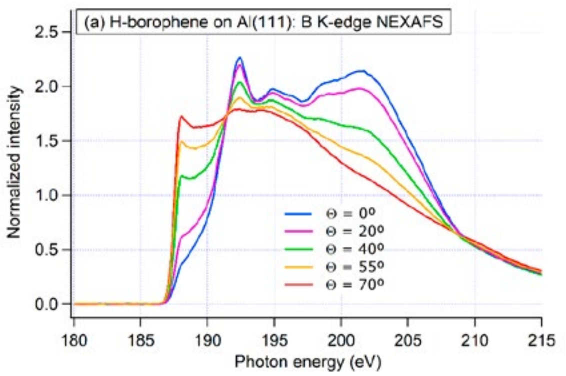
Brophene's polymorphism has raised new interest in 2D boron sheets as scientists discovered first stable borophene allotropes on Ag(111). Borophene is a promising material for various technological applications, e.g batteries and supercapacitors, sensors, and catalysis.

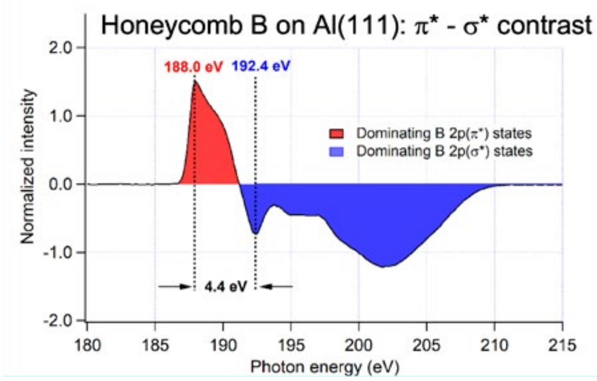
Researchers found that although honeycomb boron formed on Al(111) does resemble graphene in electronic structure to some extent, it fails to form a quasi-freestanding monolayer on aluminum. The honeycomb boron essentially matches the metallic substrate so closely that it let the topmost Al layer expand relative to the bulk and form a flat two-dimensional compound AlB_2. Therefore, the honeycomb borophene cannot be considered an independent material like graphene. If it were a structural analogue of graphene, it could wiggle like a blanket on the aluminum substrate to accommodate the small mismatch.

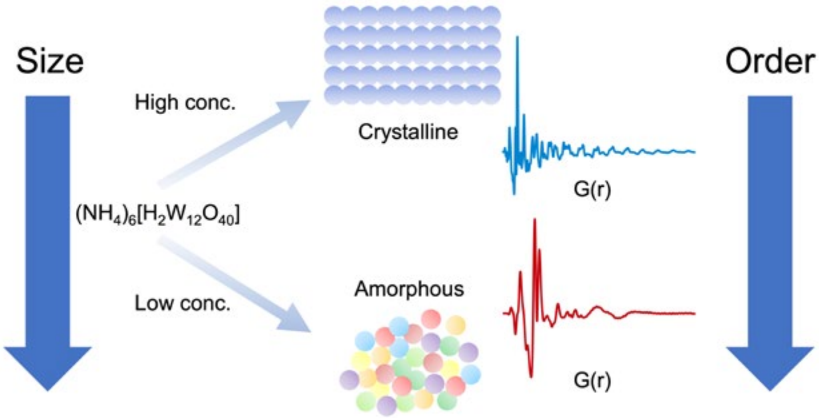
MAX IV's soft X-ray spectroscopic methods are suitable for different borophene allotropes research, as they provide direct access to the chemistry and electronic structure of these intriguing materials and allow to study their interactions with substrates and adsorbates.

Publication

A. B. Preobrajenski, et. al, Honeycomb Boron on Al(111): From the Concept of Borophene to the Two-Dimensional Boride. *ACS Nano*, 2021, 15, 9, 15153–15165. DOI: 10.1021/acsnano.1c05603







ADVANCED MATERIALS

Observing size-based nanostructure transformation

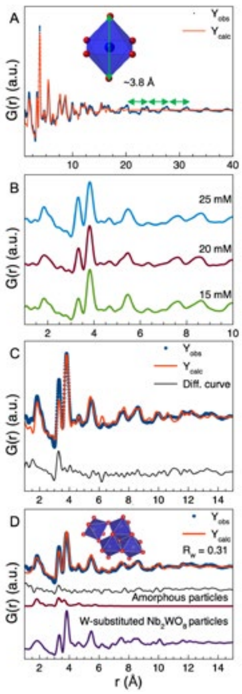
Nanomaterials play a crucial role in a broad range of applications, such as catalysis, batteries, solar cells, memory storage, medicine etc. To improve nanomaterials design for new technologies, researchers need to understand its size-structure relationship.

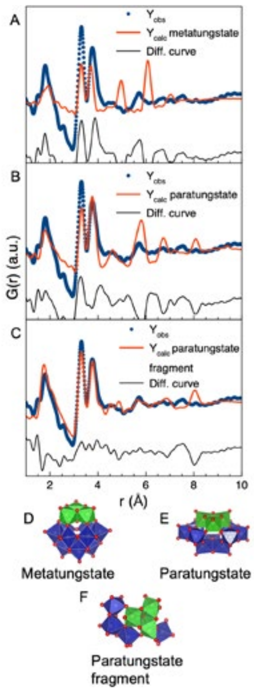
This motivated the Nanostructure group from the Dept. of Chemistry, University of Copenhagen, to investigate the influence of nanoparticles' size on their atomic structure. The research took advantage of the total scattering and pair distribution function analysis method which is available at the DanMAX beamline.

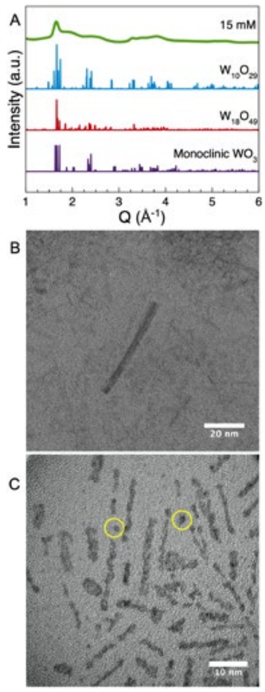
The team reported that tungsten oxide, which is usually in a crystalline structure, turned amorphous when nanosized into around 2–4 nm. It means its atomic structure changed from a repeated ordered lattice into a disordered one with no long-range atomic order.

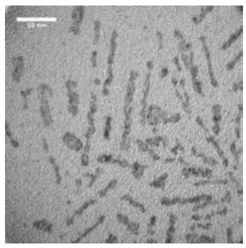
Publication

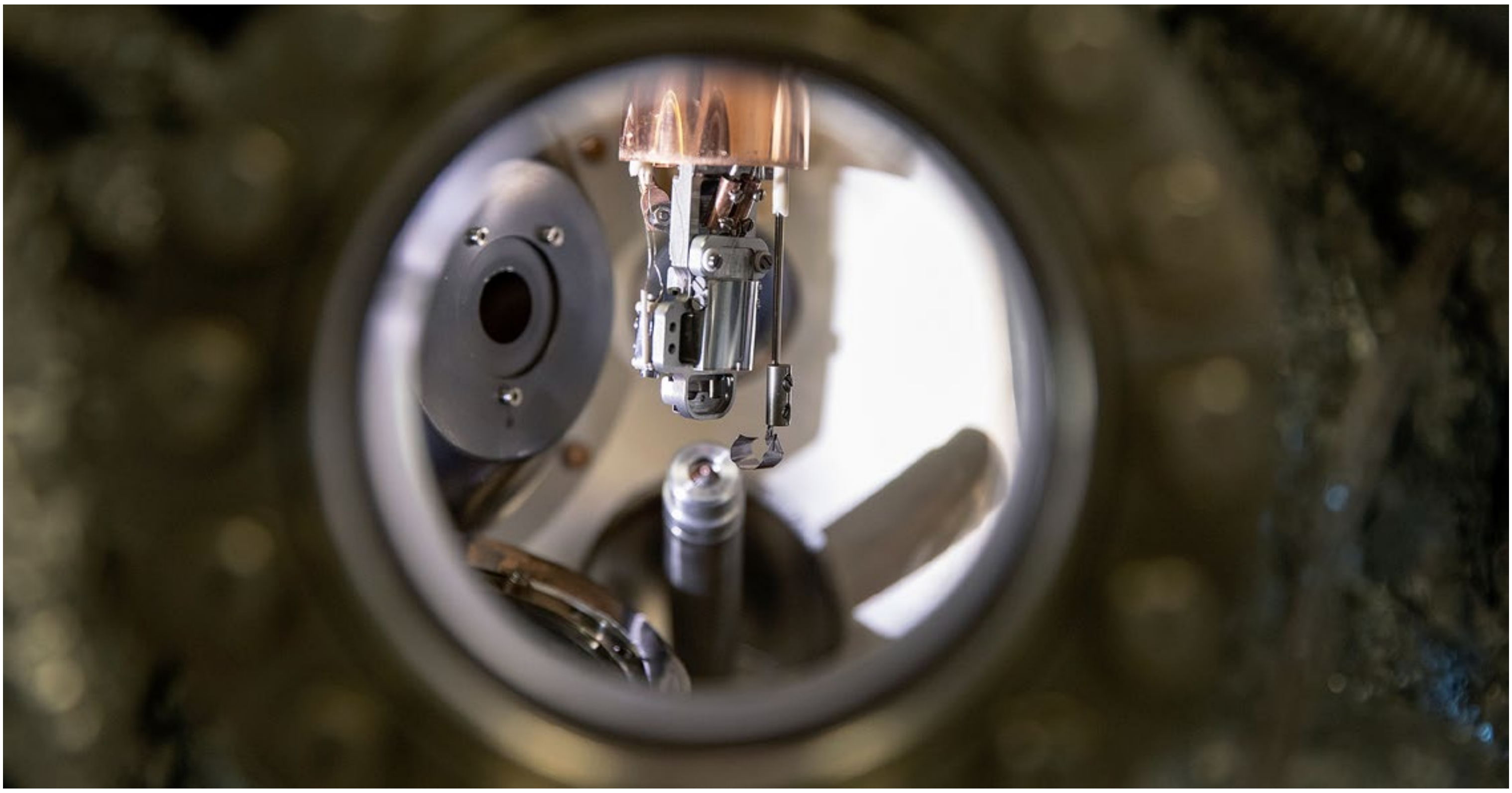
M. Juelsholt et. al, Size-induced amorphous structure in tungsten oxide nanoparticles, *Nanoscale*, 13, 20144-20156 (2021), DOI: 10.1039/D1NR05991B

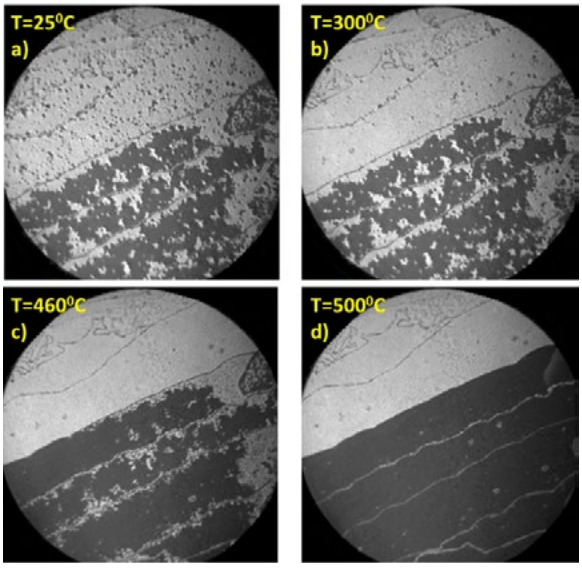












ADVANCED MATERIALS

Finding clues for future graphene-based optoelectronic devices

In-house research at MAX IV attempted to tailor epitaxial graphene's electronic structure using an advanced intercalation technique. Intercalation of germanium (Ge) is particularly interesting for its ambipolar (p- and n-) doping behavior for developing novel graphene-based optoelectronic devices.

The aberration-corrected spectroscopic photoemission and low-energy electron microscope installed at MAXPEEM beamline offer unique possibilities to simultaneously extract elemental, chemical, magnetic, and electronic information at spatial resolutions below 10 nanometer.

The research found that intercalated Ge atoms are highly mobile at the interface – a potential sign for creating ultrashort p-n junctions. This p-n boundary has a negative refractive index, which means possible applications in focusing electron optics.

Publication

Zakharov A. A., Ambipolar Behavior of Ge-Intercalated Graphene: Interfacial Dynamics and Possible Applications, *Frontiers in Physics*, 9, 2021. DOI: 10.3389/fphy.2021.641168

ADVANCED MATERIALS

One step closer to MRAM devices

Antiferromagnetic spintronics holds the development of higher operation frequencies and device's memory loss prevention, of which ferromagnetic devices suffer. However, the challenging read-out of the orientation of the staggered magnetization is a significant obstacle to harnessing the ultra-fast dynamics and stability of antiferromagnets for novel applications.

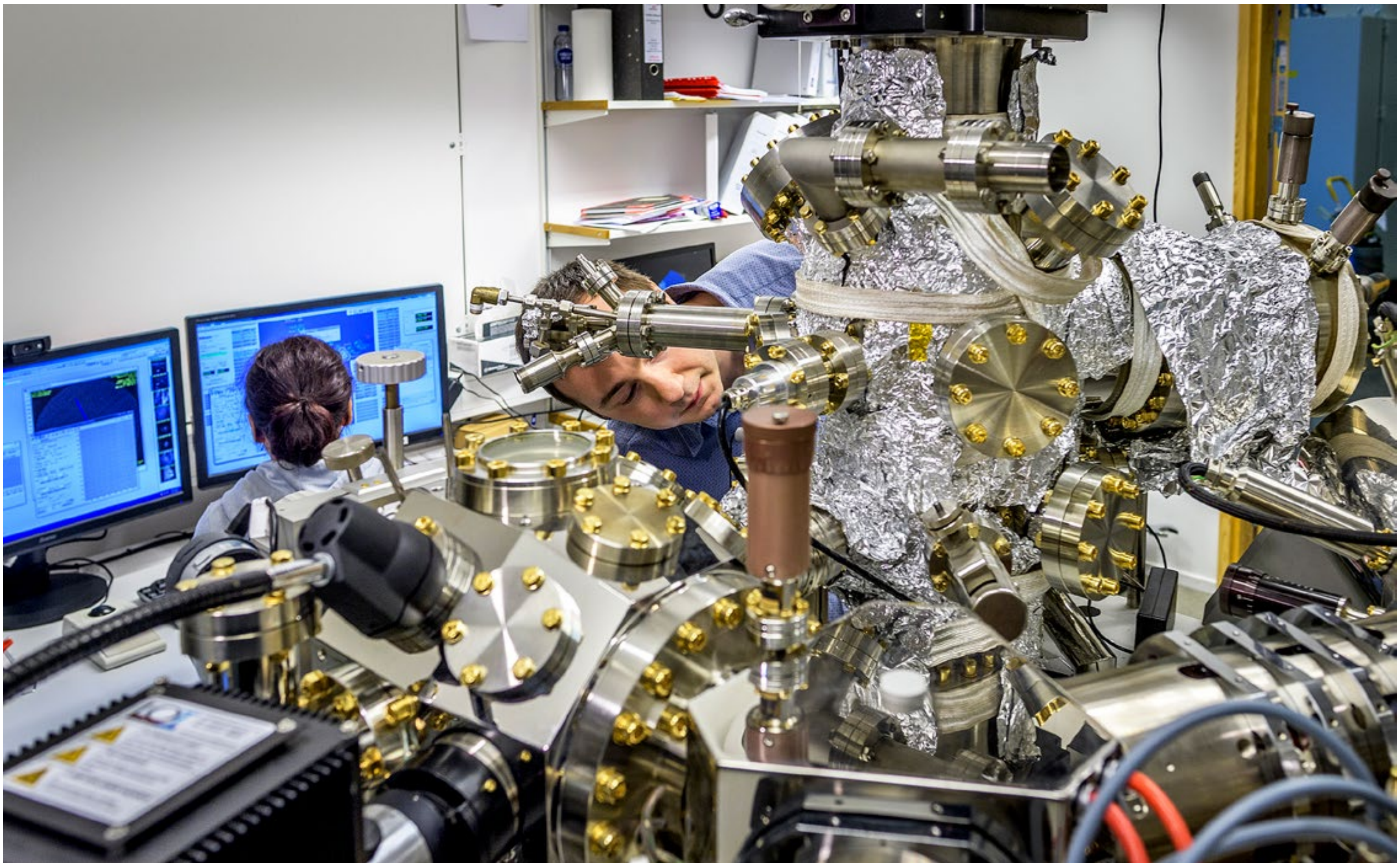
An international group of researchers from Johannes Gutenberg University Mainz, Forschungszentrum Jülich, Diamond Light Source, and MAX IV demonstrated that the coupling of the antiferromagnetic compound Manganese Gold with a thin ferromagnetic Permalloy layer was strong enough to still ensure very fast dynamics.

The coupling of the antiferromagnetic compound to the thin ferromagnet allows scientists to use any of the established technology for reading out ferromagnets on antiferromagnetic materials. The perpendicular angle of incidence and geometry at MAX IV's MAXPEEM beamline was crucial to achieving the great contrast needed in the experiment.

The long-term goal of this research is the development of much faster spintronics devices such as non-volatile magnetic random-access memory (MRAM).

Publication

Bommanaboyena, S.P., Backes, D., Veiga, L.S.I. et al. Readout of an antiferromagnetic spintronics system by strong exchange coupling of Mn2Au and Permalloy. *Nature Communications*. 12, 6539 (2021). DOI: 10.1038/s41467-021-26892-7



ADVANCED MATERIALS

Revealing N2210(OTf) electrochemical stability at positively and negatively polarised high surface area carbon material

Intrigued to know whether proton containing quaternary ammonium cation can be a source of hydrogen, the research group from Physical and Electrochemistry of the University of Tartu investigated the electrochemical stability of diethylmethylammonium triflate (N2210(OTf)) at positively and negatively polarised high surface area micro-mesoporous carbon electrodes (mmp-C(Mo_2C)), synthesised from Mo_2C.

In situ XPS (FinEstBeAMS beamline, gas-phase endstation), CV and EIS data provide excellent information about the adsorption behaviour of N2210(OTf) at carbon electrode (mmp-C(Mo_2C)) in this research.

Researchers concluded that the existence of trace water reduces the electrochemical stability of N2210(OTf) at $E < -1.30$ V (*vs*. Ag-QRE) initiating the formation of various hydrocarbon compounds and causes the formation of an insulating layer at mmp-C(Mo_2C) electrode at $E >$ 1.50 V (*vs*. Ag-QRE) probably due to the start of the trace water electrochemical oxidation and oxygen formation.

This experiment is prominent to the planning and development process of Proton Exchange Membrane Fuel Cell (PEMFCs) as it gives better information about the adsorption type and the applicable (electrochemical) potential range for the N2210(OTf) | mmp-C(Mo_2C) electrode material systems supporting the planning and development of electrolysers, electrochemical power sources, electrochemical energy storage systems (e.g. supercapacitors), metals electro-deposition and -polishing processes.

Publication

J. Kruusma et. al., The electrochemical behaviour of protic quaternary amine based room-temperature ionic liquid N2210(OTf) at negatively and positively polarized micro-mesoporous carbon electrode investigated by *in situ* X-ray photoelectron spectroscopy, *in situ* mass-spectroscopy, cyclic voltammetry and electrochemical impedance spectroscopy methods, *Journal of Electroanalytical Chemistry*, Volume 897, 2021, 115561, DOI: 10.1016/j.jelechem.2021.115561

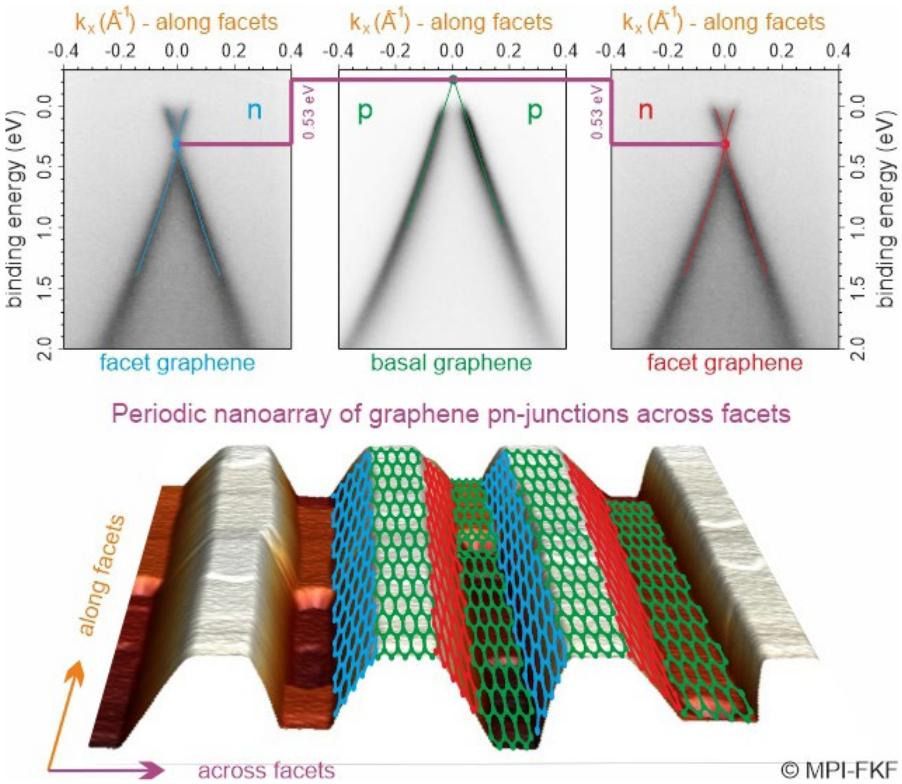
ADVANCED MATERIALS

Structuring graphene for scalability in optoelectronics

Graphene pn-junctions are envisioned as promising components of future optoelectronic and spintronic technologies. A study by researchers at Max Planck Institute for Solid State Research outlines a precision structuring method that could enable the scalable manufacturing of periodic nanoarrays of graphene pn-junctions on semiconductor silicon carbide (SiC) substrates. In the experiment, 1-dimensonally confined epitaxial armchair graphene nanoribbons (AGNRs) were converted to a 2-dimensional graphene carpet over a SiC substrate, via the insertion method, hydrogen intercalation. Results showed the product had an expected 2D-graphene electronic structure with the typical graphene pi-band dispersion, and a periodic array of p-doped (hole carriers) and n-doped (electron carriers) stripes, with junction interfaces sharper than achievable with conventional gating techniques. The electronic structure of the hydrogen intercalated graphene was analyzed at MAX IV's BLOCH beamline by Angle-Resolved Photoelectron Spectroscopy (ARPES), including doping levels and graphene orientation. The work holds promise for the development of novel optoelectronic devices such as sensors, beam splitters, or those utilizing Klein tunnelling or Veselago lenses, for example.

Ref:

H. Karakachian et al. Periodic Nanoarray of Graphene pn-Junctions on Silicon Carbide Obtained by Hydrogen Intercalation. *Adv. Funct. Mater*. 2022, 32, 2109839. DOI: 10.1002/adfm.202109839



ADVANCED MATERIALS

Relationship between defects and magnetic domains in an antiferromagnet

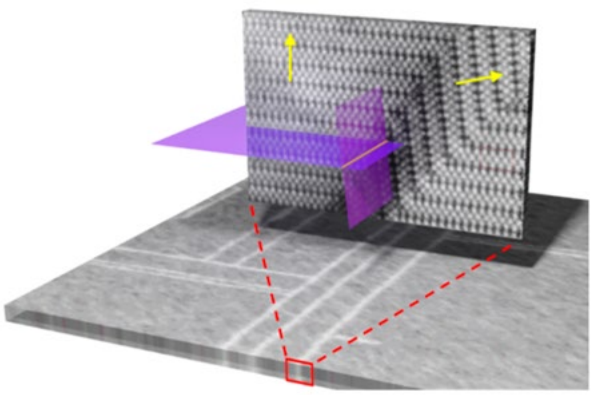
Antiferromagnets possess a magnetic order without producing a magnetic field. This characteristic is advantageous for the development of magnetic memory devices, but also means it is very challenging to measure their magnetic structure, particularly for thin films and surfaces. The mechanisms governing the formation of magnetic domains in antiferromagnetic thin films are largely unexplored.

This study explores the relationship between crystal defects and magnetic structure in thin films of the antiferromagnet, CuMnAs. This material could form the basis of future multi-state memory devices, which could function like neurons in the brain for next-generation computing technologies.

The researchers used a variety of X-ray methods with Scanning X-ray Diffraction Microscopy performed at NANOMAX. The study showed that a particular type of defect, consisting of a thin slab of a rotated phase of the crystal, can have a huge effect on the magnetic domains. The defects can fully determine the shape of magnetic domains and the location and orientation of their boundaries.

Publication

S. Reimers, Defect-driven antiferromagnetic domain walls in CuMnAs films, Nat. Commun. 13, 724 (2022), DOI: 10.1038/s41467-022-28311-x



ADVANCED MATERIALS

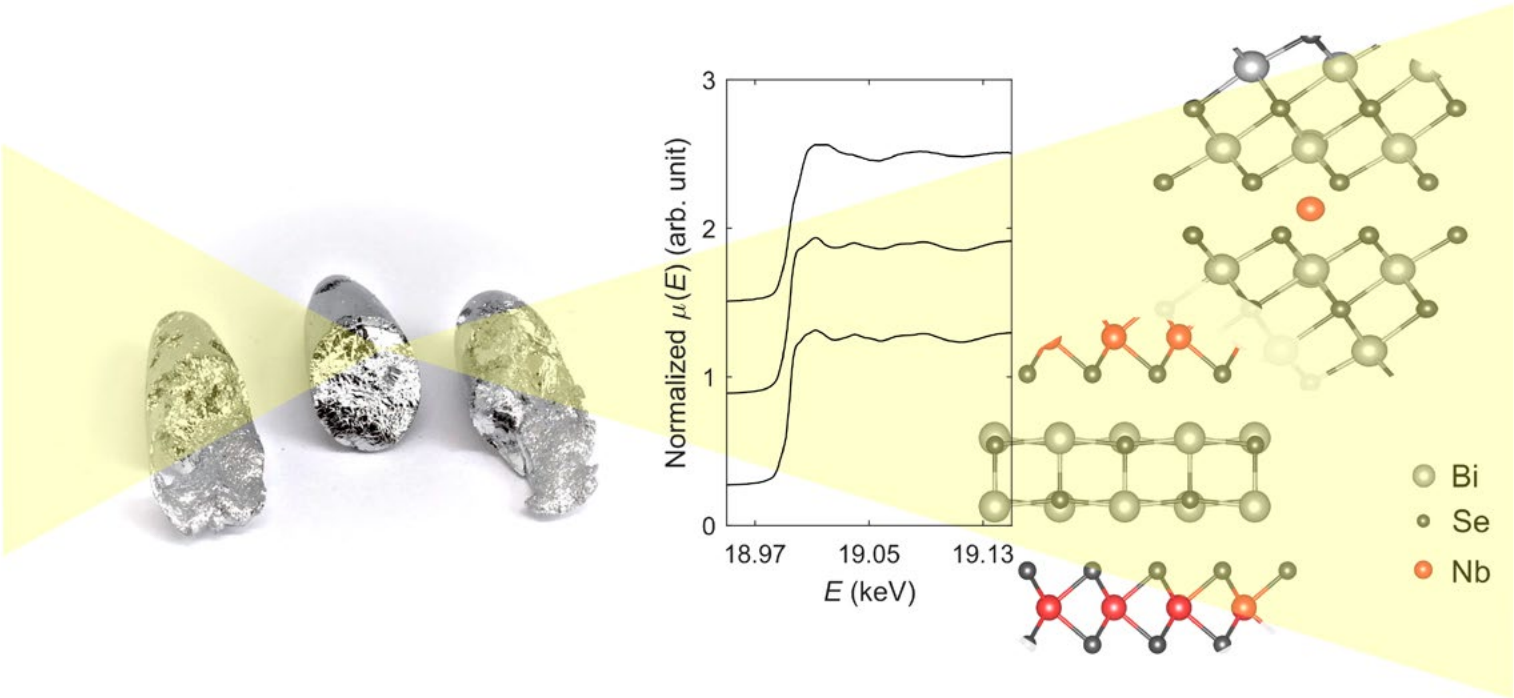
The structure of topological insulator superconductivity

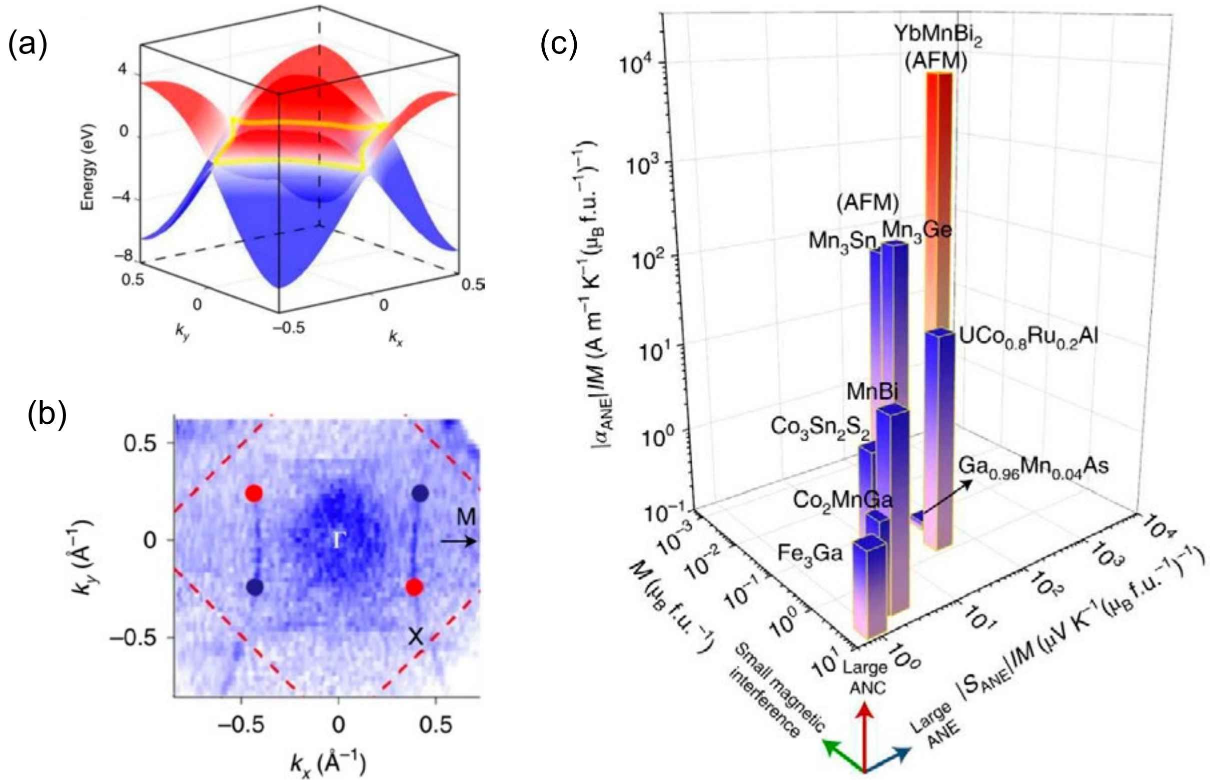
Superconductivity in topological insulators like Bi2Se3 is of high scientific interest, due to their potential to host novel quasi-particles, which are an important ingredient in proposed quantum computing technologies. In the past decade, it was discovered that Nb, Cu and Sr doping in Bi_2Se_3 induces a superconducting transition. However, thorough structural studies of these systems are scarce, although the structural characteristic is the key to understand the mechanism of the emerging superconducting properties.

A team led by researchers from Aarhus University has studied the local structure of superconducting Nb-doped Bi2Se3 using powder X-ray diffraction (PXRD) and X-ray absorption fine structure spectroscopy (XAFS). They found that contrary to common belief the origin of the superconductivity can be explained by the presence of a secondary phase, $(BiSe)_{1+\delta}NbSe_2$, rather than a Bi_2Se_3 with Nb intercalated into the van der Waals gap. The finding will make a solid foundation for progress in the field of topological superconductivity in particular and doping-induced physical properties in general.

Publication

K. Junker Dalgaard et al., Local structure of Nb in superconducting Nb-doped Bi_2Se_3, Phys Rev B, 103, 184103 (2021), DOI: 10.1103/PhysRevB.103.184103





ADVANCED MATERIALS

Nernst effect for successful thermoelectrics

A thermoelectric generator can generate electrical energy from a temperature gradient in for example an engine. Standard thermoelectric materials used works with the Seebeck effect and needs more than one material in combination to work. Instead using the Nernst effect, present in certain materials, would greatly facilitate fabrication with only one material needed in the device.

Researchers from Max Planck institute for Chemical Physics of Solids have investigated the anomalous Nernst/Hall effects in a non-collinear antiferromagnet $YbMnBi_2$. Despite an extremely low magnetisation, anomalous Nernst conductivity of 10 A/mK is achieved. The work demonstrates the great potential of noncollinear antiferromagnets, beyond general ferromagnets, for transverse thermoelectric applications. Antiferromagnets have many advantages and broadens the spectrum of potential materials.

The experiment was performed using Angle Resolved Photoelectron Spectroscopy (ARPES). The analyser used works in deflector mode, which allows us to map the Fermi surface of the whole Brillion zone without tilting the sample, and therefore ensures the ARPES spectra are acquired from the same region.

Publication

Y. Pan et al., Giant anomalous Nernst signal in the antiferromagnet YbMnBi2, Nature Mat. 21, 203 (2022), DOI: 10.1038/s41563-021-01149-2

ADVANCED MATERIALS

Properties of heavy electrons clue to peculiar superconductivity

A team led by researchers from Zhejiang University have studied how the electrons behave in the heavy fermion superconductor $CeCu_2Si_2$ using Angular Resolved Photoelectron Spectroscopy (ARPES). The superconductivity of $CeCu_2Si_2$ cannot be explained with the standard Bardeen-Cooper-Schrieffer model.

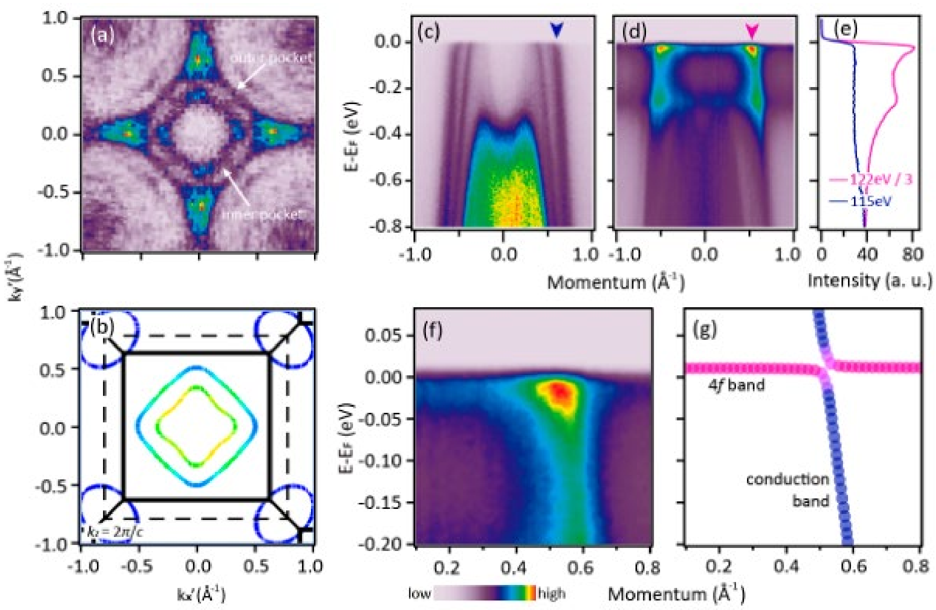
The heavy electrons were found to have very different properties at different locations in momentum space: at some places, they form quasi-2D cyclindral shape bands, while in other momentum places, they are more three-dimensional. Such a large momentum anisotropy can be important to get a picture of its peculiar superconductivity.

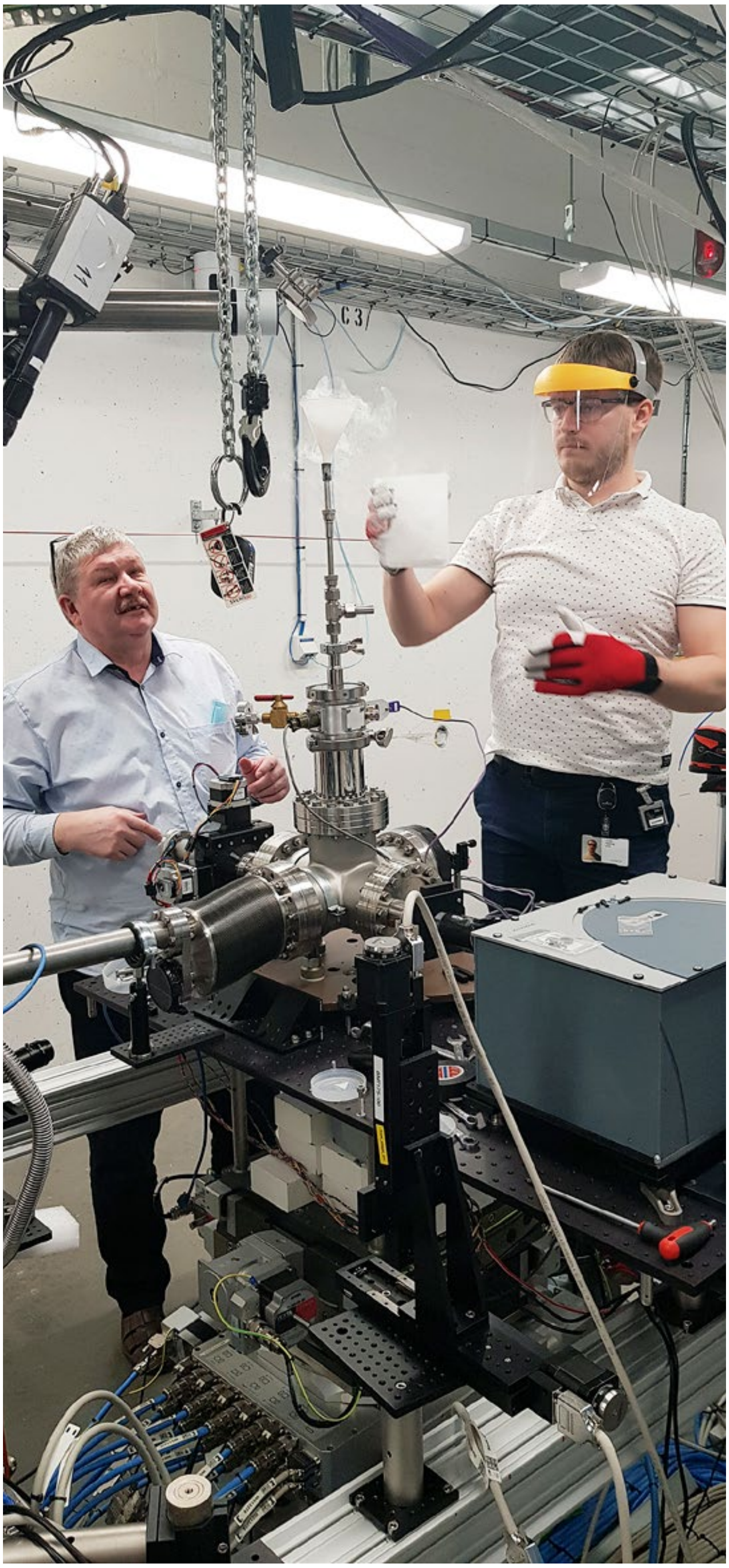
Understanding how such many-body interaction arises and evolves is very important for understanding many exotic properties in solid state physics, such as high temperature superconductivity and colossal magnetoresistance.

This is the first successful attempt to measure the dispersive electron bands in momentum space for $CeCu_2Si_2$. The small beam size and high photon flux at BLOCH beamline made it possible.

Publication

Z. Wu et al., Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor $CeCu_2Si_2$, Phys. Rev. Lett. 127, 067002 (2021), DOI: 10.1103/PhysRevLett.127.067002





ADVANCED MATERIALS

Novel scintillator materials for fast timing applications

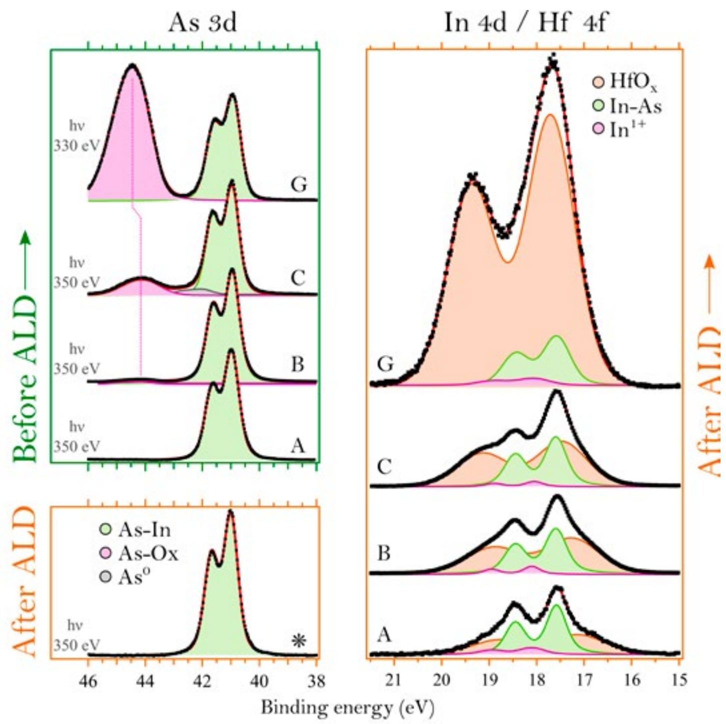
Scintillators with excellent time resolution are needed in medicine, high-energy physics experiments and other fast timing applications. Time-of-flight positron emission tomography (TOF-PET) is a medical diagnostic imaging modality where the time resolution of the detection system, including the scintillator affects the signal-to-noise ratio of the diagnostic image used to detect tumours.

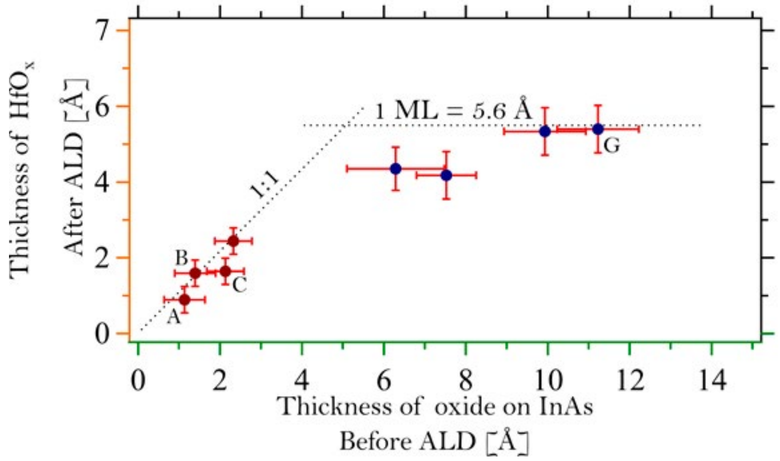
A team led by researchers from University of Tartu has studied ultrafast relaxation processes of electronic excitations, leading to intrinsic emissions such as cross-luminescence and intraband luminescence in potential scintillator materials. The researchers conducted time-resolved photoluminescence experiments. Time-resolved emission and excitation spectra as well as decay curves of various emission were recorded for several ternary hexafluoride powders in single-bunch operation mode.

The results of this study contribute to developing new scintillator materials to be used in fast timing applications. The work demonstrates the potential of the band structure engineering concept in the development of new luminescence and optical materials. It also shows how important the improvement of the limits of time-resolved experimental methods are, which can be applied in scintillator research using a full potential of synchrotron radiation sources.

Publication

J. Saaring et al., Relaxation of electronic excitations in K2GeF6 studied by means of time-resolved luminescence spectroscopy under VUV and pulsed electron beam excitation, J. Alloys Compd. 883, 160916 (2021), DOI: 10.1016/j.jallcom.2021.160916





ADVANCED MATERIALS

Oxygen relocation during HfO_2 ALD on InAs

In a study led by researchers from Lund University, the atomic layer deposition (ALD) of HfO_2 on InAs and the influence of the original surface oxide layer present was investigated. ALD, a technique that is widely used in industry, is studied in real-time with ambient pressure X-ray Photoelectron Spectroscopy (AP-XPS).

Until now, the surface chemistry behind this deposition approach has been modeled based on indirect observations, resulting in the so-called ligand exchange model with the main assumption that the reaction is not influenced by the original surface. The study shows that this assumption is wrong during the initial phase of the ALD reaction. Importantly, it is this initial phase which determines the quality of the final material interface.

The results of the study contributes to the development of next-generation electronics as well as the understanding of the ALD method itself through the unique experimental setup at beamline SPECIES.

Publication

G. D'Acunto et al., Oxygen relocation during HfO_2 ALD on InAs, Faraday Discuss 236, 71 (2022), DOI: doi.org/10.1039/D1FD00116G

ADVANCED MATERIALS

Revealing mechanical properties of ferroelastic perovskites

Metal halide perovskites are important for many applications, ranging from solar cells to opto-electronic devices. However, defects and crystal inhomogeneities can affect their optical and electronical properties, significantly reducing their efficiency.

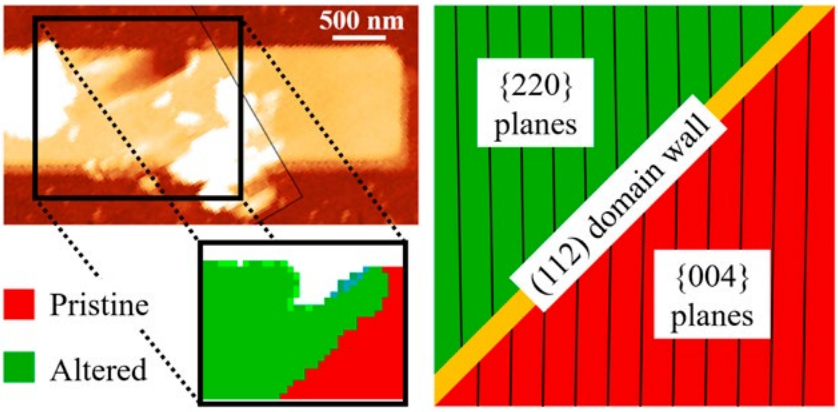
The focus of the study led by reserachers from Lund University was to demonstrate the formation of ferroelastic domains in metal halide perovskite $CsPbBr_3$ nanowires under external load. They used an atomic force microscope tip to induce local pressure on the nanowires, and the 60 nm focused X-ray beam at NanoMAX as a probe. The lattice spacing and tilt along the structures could be imaged with high resolution.

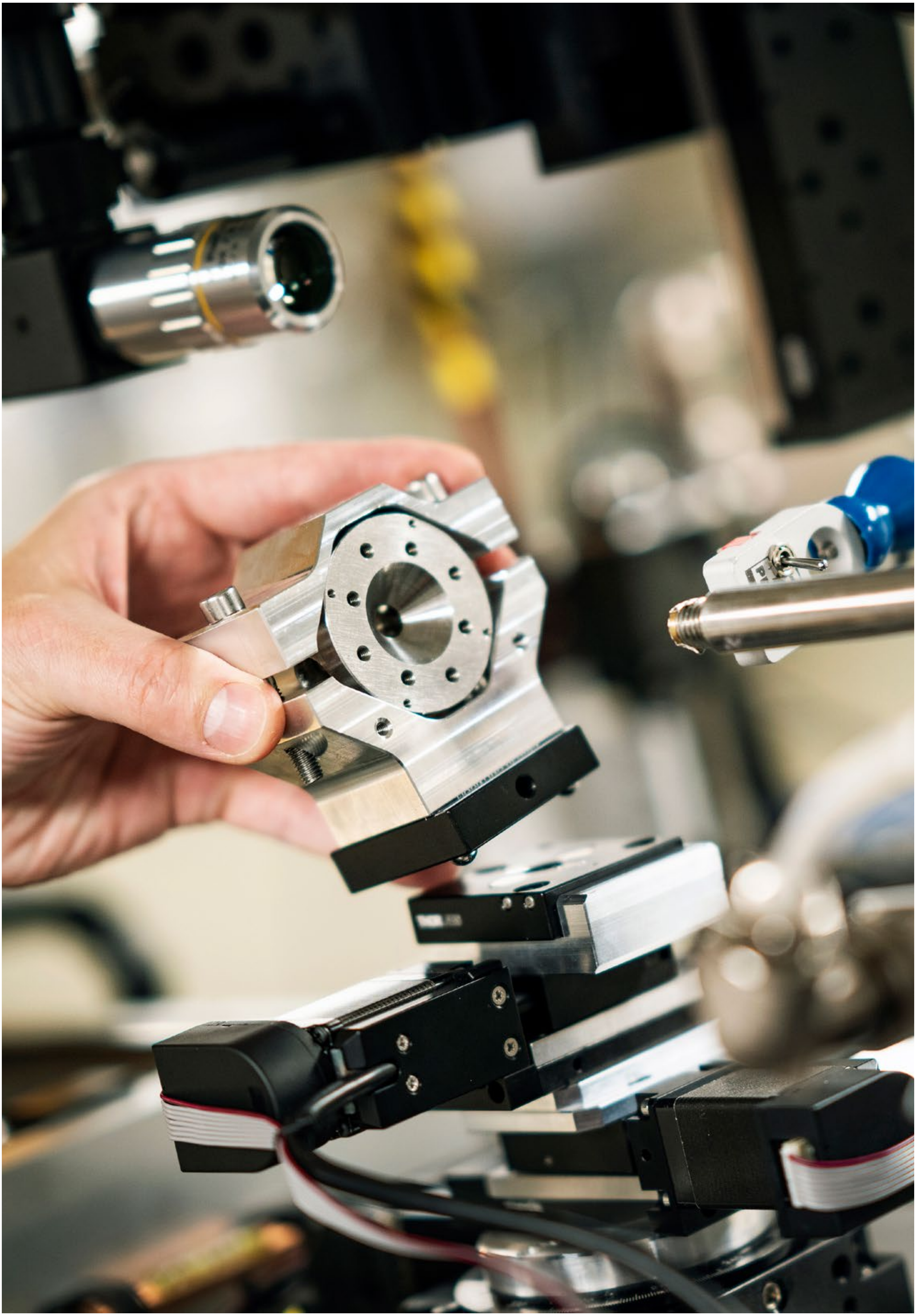
The researchers managed to unambiguously determine the crystal structure at manipulated and pristine domains, revealing their ferroelastic nature.

The study revealed new properties of $CsPbBr_3$ nanostructures. From the basic materials properties point of view, this is a knowledge step on halide perovskites for the materials science community. For the applied science side, the findings help clarifying so far unknown mechanical properties of this material, which might directly affect their usability on for example new generation X-ray detection devices.

Publication

L. A. B. Marçal et al., Inducing ferroelastic domains in single-crystal CsPbBr3 perovskite nanowires using atomic force microscopy, Phys. Rev. Materials 5, L063001 (2021), DOI: 10.1103/PhysRevMaterials.5.L063001

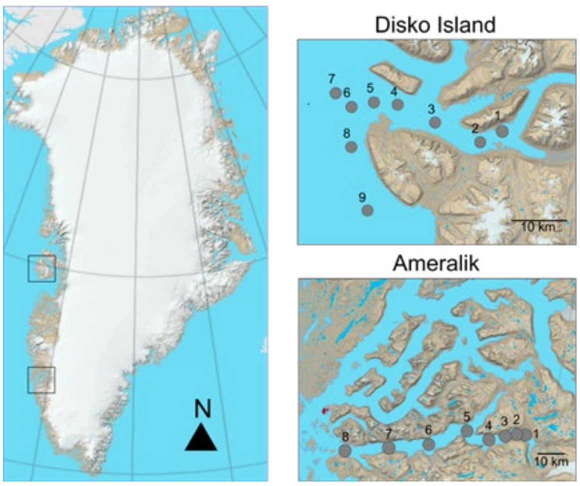




ENVIRONMENTAL SCIENCE

Diving into Greenlandic glacial rock flour

The warming arctic air temperatures increase the flux of glacial rock flour to fjords and coastal regions due to the melting of the Greenland Ice Sheet. The particles' biogeochemical reactivity can be a source of trace metals and macronutrients that enhance marine phytoplankton growth.



Researchers from the Geochemistry Department of the Geological Survey of Denmark and Greenland thus investigated the solid-phase Fe speciation in suspended sediment collected from four West Greenlandic fjords of up to 100 km. The Balder beamline's fluorescence detectors and X-ray flux were crucial to performing X-ray absorption spectroscopy on these natural particles, in addition to physical oceanography data and aqueous chemical measurements.

Researchers found that the type of host phase for Fe in the suspended particles varied depending on the underlying geology of the fjords. Surprisingly, the solid-phase Fe speciation of suspended particles was generally unchanged along the length of large fjords and with depths exceeding 300 m. They also found that the fjord dFe levels were unrelated to the dominant type of solid-phase Fe.

Publication

C.M. van Genuchten et. al, Decoupling of particles and dissolved iron downstream of Greenlandic glacier outflows, *Earth and Planetary Science Letters*, Volume 576, 2021, 117234, DOI: 10.1016/j.epsl.2021.117234.

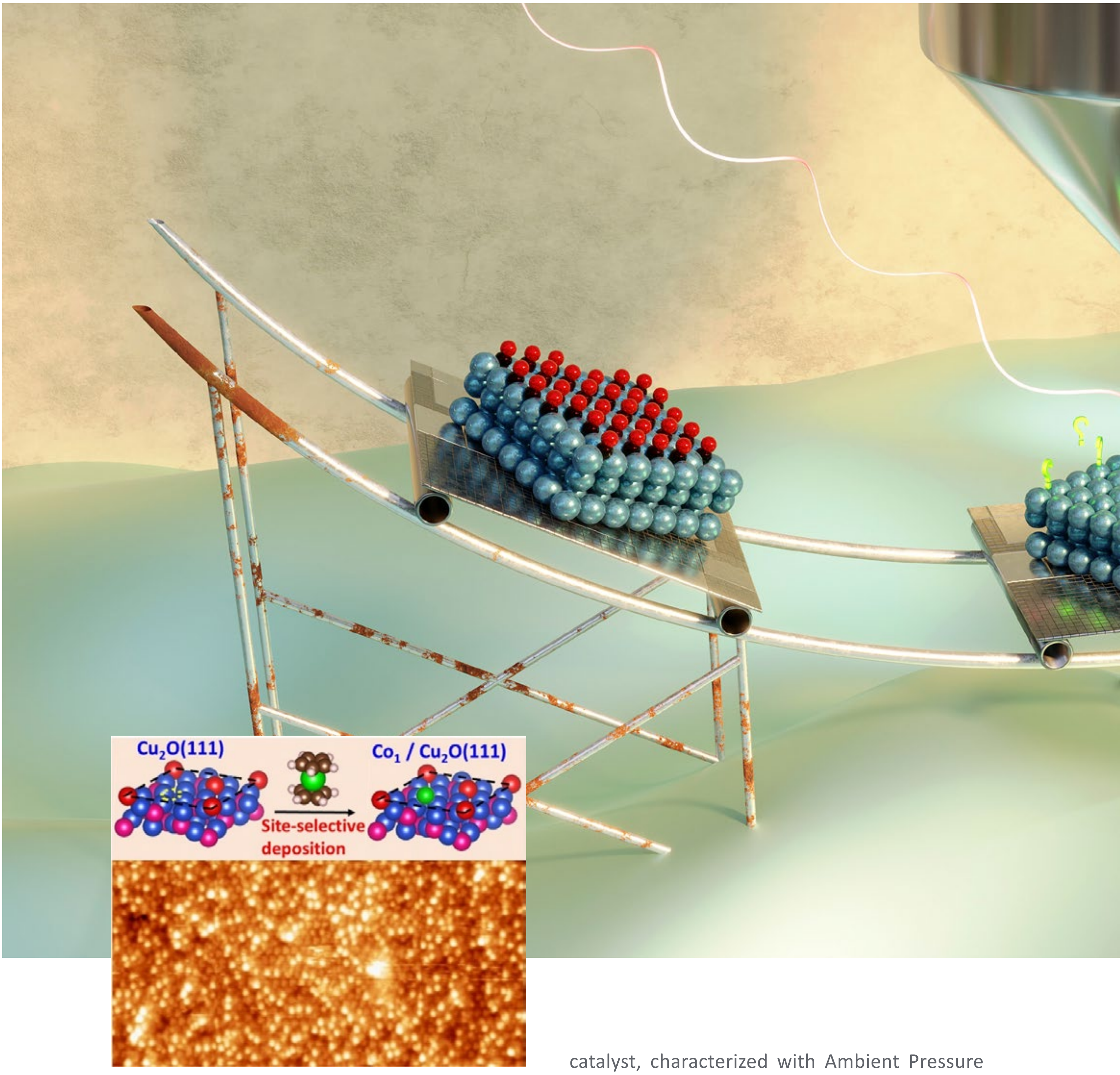
ENVIRONMENTAL SCIENCE

Earth salts aid understanding of Martian salt chemistry

An international study on the surface chemistry of Earth salts has captured new insights of the Martian atmospheric chemistry and climate system. Researchers from the University of Gothenburg in Sweden used HIPPIE beamline to characterise salt crusts, lakebed salts, and brines from two saline lakes in the Qaidam Basin in China. Results showed that the salt analogue is more sensitive than expected as the ions are fully solvated at very low relative humidity, and therefore never dry on Earth or Mars. The chemistry of solvated surfaces, including salts, plays a role in varied gas formation and secondary aerosol particle formation that directly influence the air quality and climate. The work furthers our understanding of the salt-vapor interaction—a process important in both planetary climate systems and human health.

Ref:

X. Kong et al. Surface solvation of Martian salt analogues at low relative humidities.
Environ. Sci.: Atmos., 2022, 2, 137-145.
DOI: 10.1039/d1ea00092f



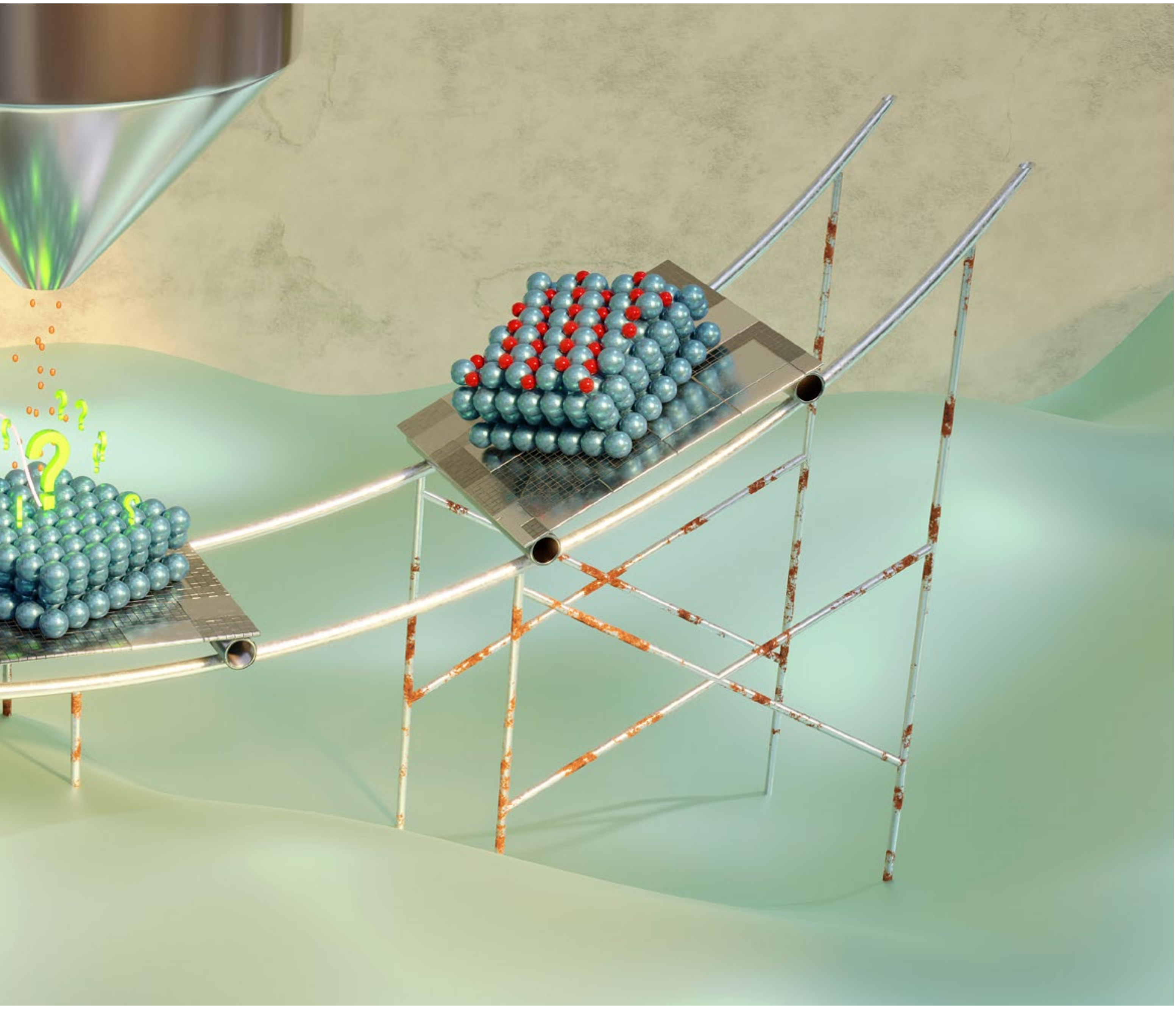
CATALYSIS

Designing stable copper catalysts for the future

Copper-based (Cu) catalysts are a promising alternative for the future replacement of noble metal catalysts. However, a known issue, the deactivation of the active Cu^+ sites during a reaction, has hindered commercial application. A study from Kungliga Tekniska Högskolan in Sweden used atomic layer deposition to grow a single-atom Co_1Cu alloy on the surface of a copper oxide support. The resulting hybrid single-atom catalyst, characterized with Ambient Pressure XPS at the HIPPIE beamline, exhibited a remarkable stabilization of the Cu^+ surface sites while simultaneously maintaining a high exposure of the Cu^+ active catalytic centers to gas phase reactants. The findings offer promise for new designs of copper-based catalysts and their widespread use for industrial applications.

Ref:

C. Wang et al. Stabilization of Cu2O through Site-Selective Formation of a Co1Cu Hybrid Single-Atom Catalyst. *Chemistry of Materials* 2022 ***34*** (5), 2313-2320. DOI: 10.1021/acs.chemmater.1c04137



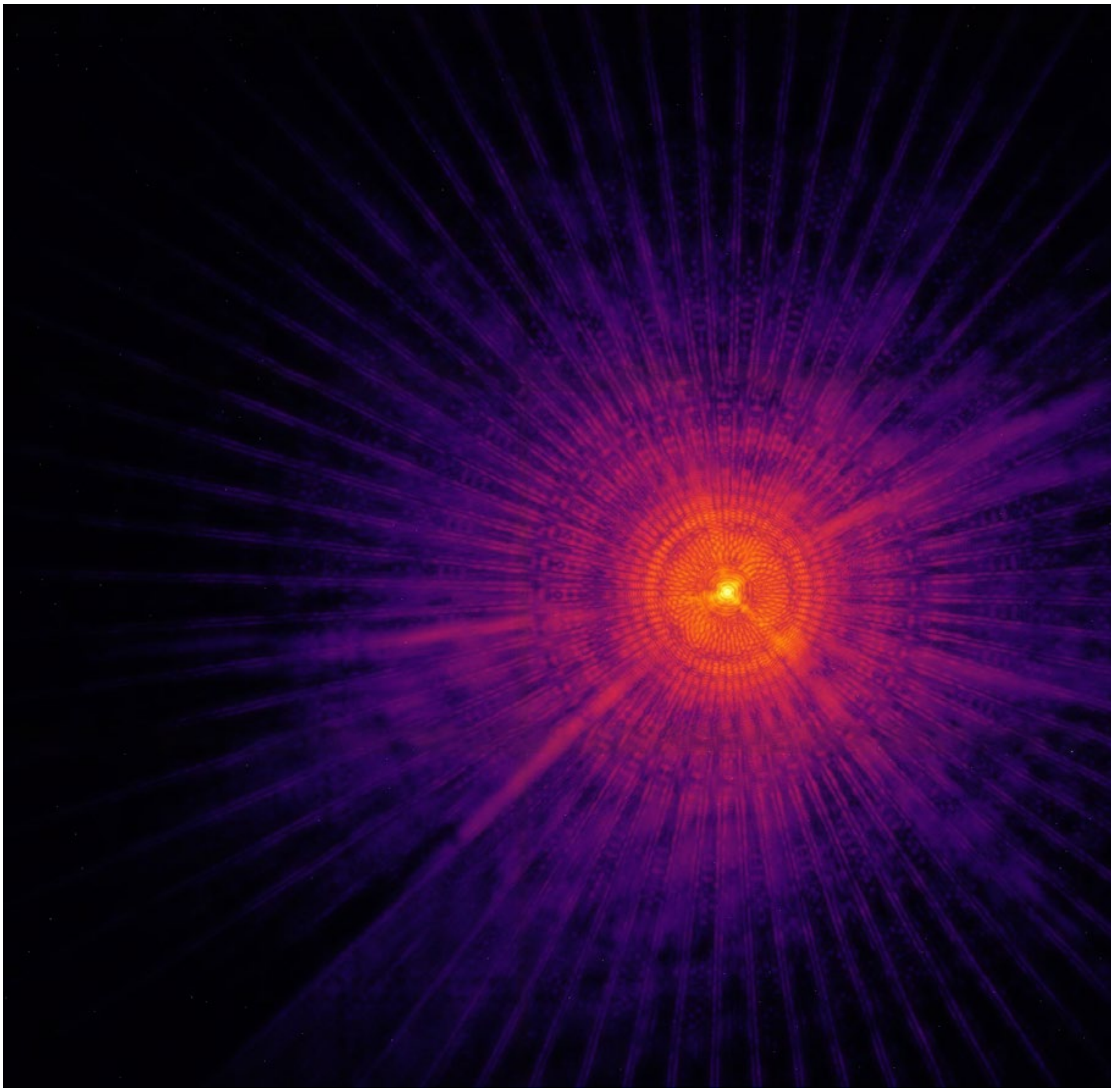
CATALYSIS

Mapping catalysis structure and conditions during a reaction

A key challenge of catalyst research is understanding how catalyst structure and function work dynamically, under local conditions of temperature, pressure, and gas, to produce a reaction. A research group from Sweden and Norway has developed a new event-averaging-based method employing time-resolved Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) to map catalyst structure and local gas environment simultaneously during rapidly changing reaction conditions. With this new method, scientists can determine in detail what triggers structural changes on the sample surface and even measure the activity during a structural transition. The experiment was conducted in part at MAX IV's HIPPIE beamline, which provided the important capability of rapid gas exchange in the sample cell, enabling the use of gas pulsing to circumvent the typically slow-paced spectrum recording of the APXPS method.

Ref:

J. Knudsen et al. Stroboscopic operando spectroscopy of the dynamics in heterogeneous catalysis by event-averaging. *Nat Commun* 12, 6117 (2021). DOI: 10.1038/s41467-021-26372-y



INSTRUMENTATION

Confirmed: CoSAXS beamline takes the research world further

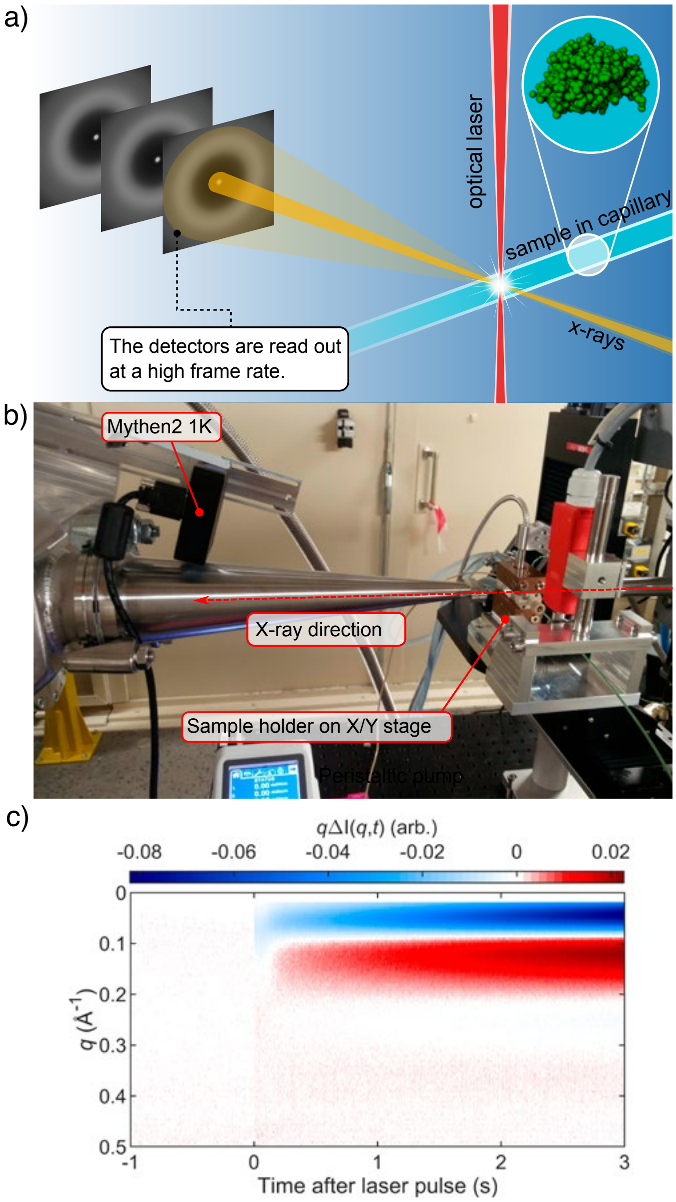
As the world's 4th generation source, MAX IV was designed to have a higher brilliance and thus an increased coherent fraction of the beam provided at its beamlines. The degree of coherence at the (then new) CoSAXS beamline, predicted in its design, needed to be confirmed.

A joint effort from CoSAXS, NanoMAX, Balder, ForMAX, and KITS team at MAX IV verified the performance parameters of the CoSAXS beamline. The team showed the CoSAXS beamline's abilities: to choose the degree of coherence as predicted by simulations, to operate the detector at the highest frame rate and to perform quantitative coherent small-angle X-ray scattering (SAXS) experiments (e.g XPCS).

With the higher coherent fraction of the beam provided at the CoSAXS beamline, new experimental limits can be reached: the detection of fainter signals, the exploration of smaller length scales and shorter time scales (faster processes). The operational stage of the CoSAXS beamline furthers the opportunity to perform the envisioned sophisticated experiments at MAX IV.

Publication

M. Kahnt et.al, Measurement of the coherent beam properties at the CoSAXS beamline, *J. Synchrotron Rad* 28, 1948–1953 (2021), DOI: 10.1107/S1600577521009140



INSTRUMENTATION

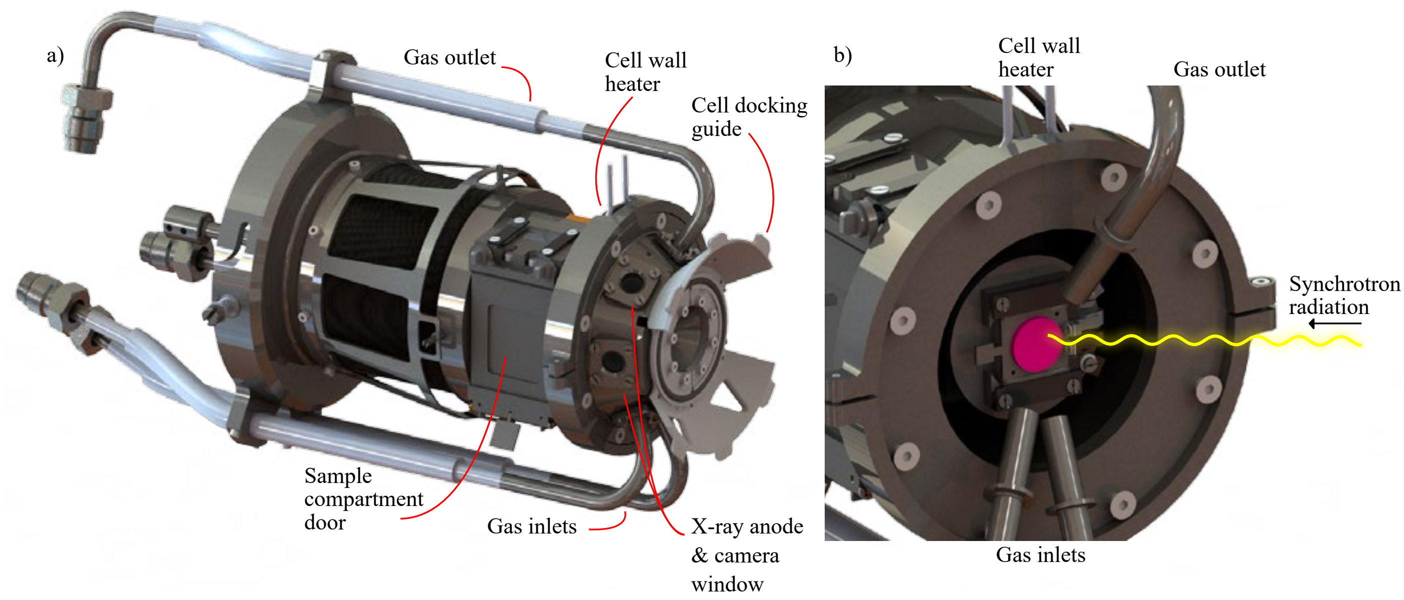
Establishing time-resolved X-ray solution scattering with milliseconds resolution at CoSAXS beamline

Various processes in physics, chemistry, or biology are naturally dynamic. Therefore, a technique that allows following structural changes in short time as a response to external perturbations is crucial. A binational collaboration between Gothenburg University, Lübeck University, Petra III and MAX IV aimed to establish a setup for performing time-resolved X-ray solution scattering experiments (TR-XSS) at the CoSAXS beamline at MAXIV laboratory.

Researchers used laser-induced temperature jumps to trigger structural changes in a protein (lysozyme) and utilized X-ray solution scattering to monitor these changes, for which the high X-rays photon flux and the simultaneous SAXS/WAXS data collection of the beamline was required. Researchers also synchronized the IR laser trigger with the X-ray data collection for the experiment. This showcases the CoSAXS beamline's capabilities to perform TR-XSS.

Publication

O. Berntsson, et. al, A setup for millisecond time-resolved X-ray solution scattering experiments at the CoSAXS beamline at the MAX IV Laboratory. *J. Synchrotron Rad.*, 29, 555-562 (2022).
DOI: 10.1107/S1600577522000996



INSTRUMENTATION

Ambient pressure X-ray photoelectron spectroscopy setup for synchrotron-based in situ and operando atomic layer deposition research

Atomic Layer Deposition, ALD, is a technique for creating highly uniform thin films. It relies on cyclically exposing the substrate surface to consecutive pulses of gases to create the desired layers.

Most studies so far have been done with the ALD reactor being physically separated from the XPS instrument, due to strict vacuum requirements in XPS instruments. In this new setup, we have developed a sample environment using the ambient pressure XPS as the technique. We call this setup the ALD cell and it enables the simultaneous XPS acquisition with the deposition of the atomic layers.

During the commissioning period of the cell, several experiments were conducted to test its performance such as deposition of TiO2 using titanium tetraisopropoxide (TTIP) and water. The results show that the technique can be used for obtaining information on the exact mechanism of the deposition process, which so far has not been so easy to obtain, especially by a surface sensitive and chemically specific technique as XPS.

We believe this cell will be a valuable addition to the beamline instruments. The cell has an impact on the development of new methods of growing these smaller and smaller structures – that are very frequently used nowadays in, e.g., micro- and nanoelectronics industries.

Publication

E.Kokkonen et al., Ambient pressure X-ray photoelectron spectroscopy setup for synchrotron-based in situ and operando atomic layer deposition research, Rev. Sci. Instr. 93, 013905 (2022), DOI: 10.1063/5.0076993

HEALTH AND MEDICINE

Multimodal imaging holds piece of the Alzheimer's puzzle

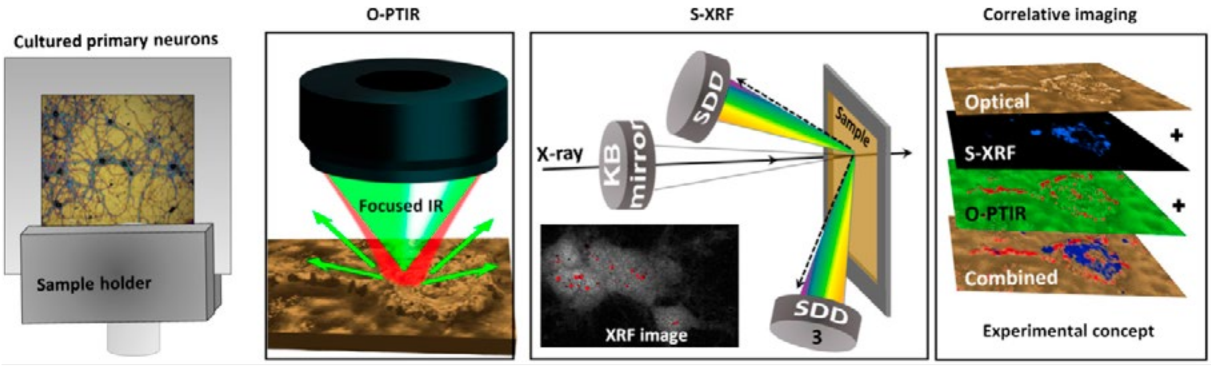
The study focuses on why beta-amyloid aggregation happens in the human brain. It is a proof of concept aimed at demonstrating the applicability of synchrotron-based techniques to study structural alterations linked to Alzheimer's disease.

The researchers carried out a proof-of-concept study which showcases that combining two imaging modalities can be effectively used in a correlative way to assess structural and chemical information directly within a single cell. They used X-ray Fluorescence to observe clustering of iron in the primary neurons. Optical Photothermal Infrared Microscopy correlates the structural changes with the iron clusters.

This correlation has not been shown before and the result opens new possibilities for further studies to understand molecular mechanisms of amyloid neurotoxicity. This, in turn, could help with understanding why the first Alzheimer's Disease changes begin and could thus – hopefully – open the doors towards developing preventative therapies for the disease.

Publication

N. Gustavsson et al., Correlative optical photothermal infrared and X-ray fluorescence for chemical imaging of trace elements and relevant molecular structures directly in neurons, Light: Science & Applications 10, 151 (2021), DOI: 10.1038/s41377-021-00590-x



ENERGY AND FUELS

Making way for blue solar cells

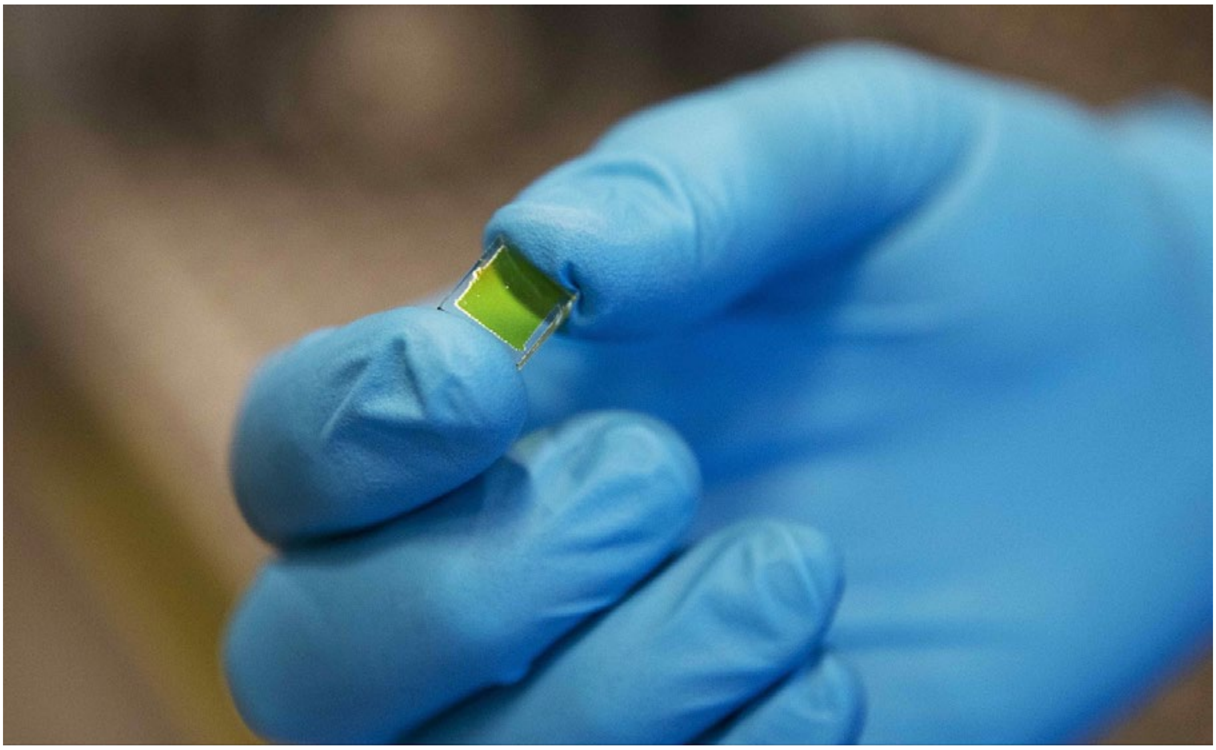
Continued work on converting solar energy into electrical or chemical energy promises more efficient applications. Characterizing bonding and charge transfer processes to the dye-sensitized solar cells' real-world efficiency is prominent in developing more efficient systems. The chemical and electronic coupling between excited electrons on the dye molecule and the conduction band of the oxide largely determines the efficiency of this process.

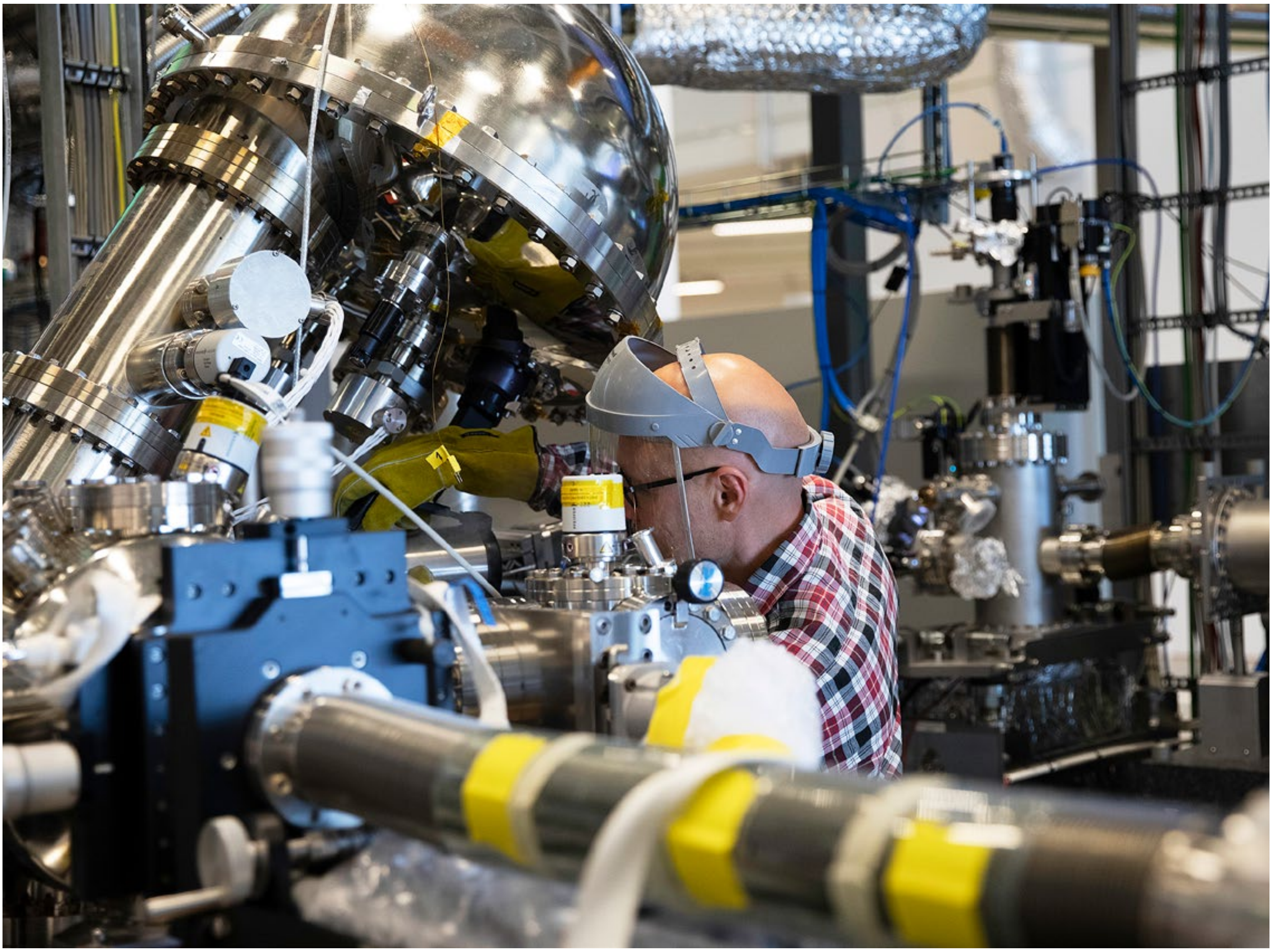
Using soft X-ray based electron spectroscopy at FlexPES beamline, scientists from the University of Nottingham characterize chemical and electronic interactions between dye molecules and oxide surfaces in light-harvesting through dye-sensitized solar cells and photocatalytic water splitting. The mesoporous titanium dioxide surfaces were sensitised with a range of trimethylamine dyes to understand the chemical bonding to the surface, electronic transitions within the molecule, and charge transfer interactions between the molecule and the oxide. X-ray photoelectron spectroscopy (XPS) was used to probe the chemical environment of each atom in the dye molecule to deduce its adsorption bonding to the surface.

This study opens ways to understand fundamental processes in dye molecules on real solar cell surfaces and potentially be applied to the study of any prospective solar cell candidate.

Publication

R.H. Temperton, et. al, A soft X-ray probe of a titania photoelectrode sensitized with a triphenylamine dye, ***J. Chem. Phys***. 154, 234707 (2021), DOI: 10.1063/5.0050531





ENERGY AND FUELS

CO adsorption on Co(0001): observing temperature and CO pressure closer

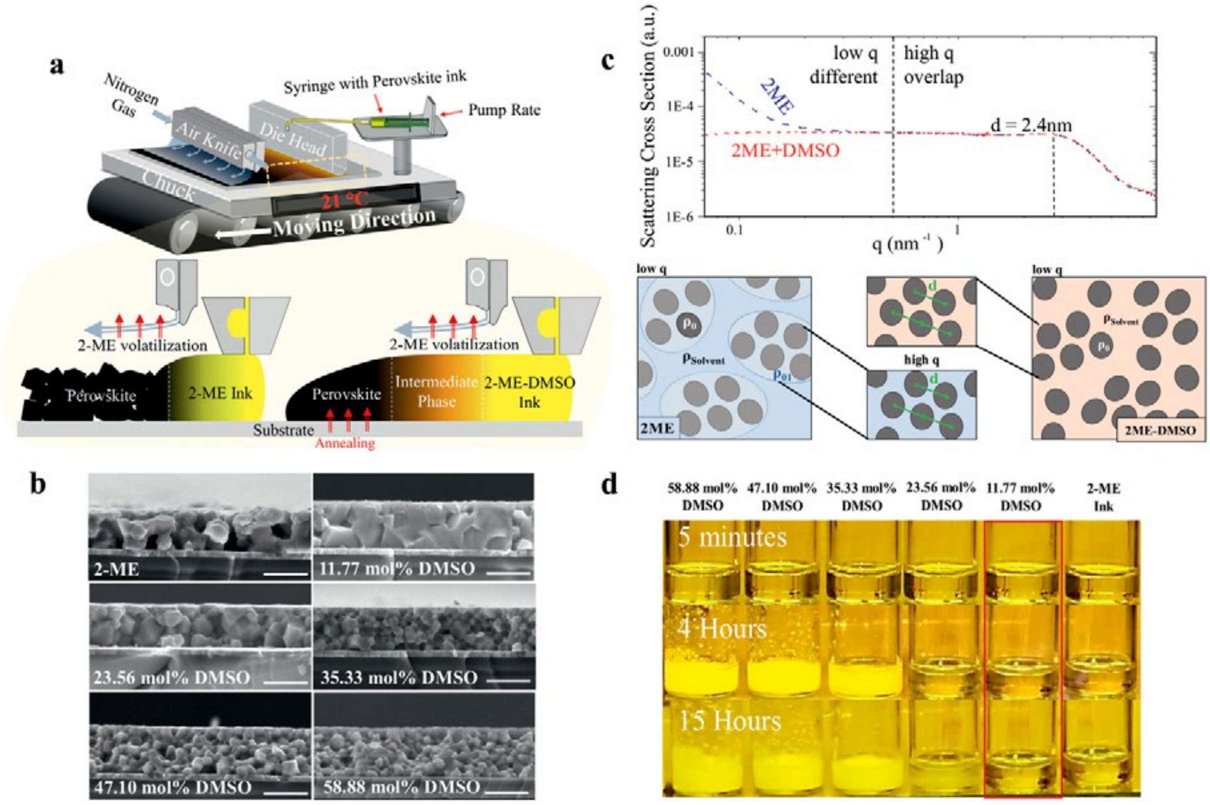
With the challenges of developing green future energy, synthetic fuels have become a potential alternative for industrial applications. Researchers from Syngaschem BV, a research company based in the Netherlands, identified new high coverage phases of CO on cobalt that were previously unknown. Cobalt catalysts can be used to produce synthetic fuels via the reaction of CO and hydrogen.

Low energy electron diffraction, XPS at FlexPES, desorption spectroscopy, and infrared absorption spectroscopy provided researchers with information about quantities and locations of the molecule on the different sites of the surface of a single crystal in ultra-high vacuum (UHV) and compared them with recently published STM images by Prof. Wintterlin group from Munich, Germany.

The result of the study is significant for catalyst characterization approaches where CO adsorption at room temperature is used as a probe to study the composition of the catalyst surface. The research provides an experimental basis for a theoretical study to observe the structural stability of two different structures based on temperature and CO pressure.

Publication

C.J. Weststrate, et. al, CO adsorption on Co(0001) revisited: High-coverage CO superstructures on the close-packed surface of cobalt, *Journal of Catalysis*, Volume 408, 2022, Pg. 142-154, DOI: 10.1016/j.jcat.2022.03.005.



ENERGY AND FUELS

Boosting processing technology for metal-halide solar cells

Researchers at Helmholtz-Zentrum Berlin and Lund University investigated the scalable solution processing technology, perovskite deposition by slot die coating (SDC), for the manufacturing of metal-halide solar cells. Results demonstrated the effect of the solvent dimethyl sulfoxide (DMSO) on the formation of the halide perovskite semi-conductor. Both the DMSO-content and age of the precursor (ink) solution used had a significant impact on the resulting morphology and quality of perovskite thin-film with application via SDC. The experiment was carried out in part at Balder beamline at MAX IV. The study furthers knowledge of ink composition and overall processing control critical for scalability of metal-halide perovskite (MHP) semiconductors, important components of optoelectronic devices such as lasers, LEDs, and detectors. Further, it provides a path for enabling high-quality halide perovskite thin films needed for commercial solar cell technology based on MHP semiconductor devices.

Ref:

Ref: J. Li et al, 20.8% Slot-Die Coated $MAPbI_3$ Perovskite Solar Cells by Optimal DMSO-Content and Age of 2-ME Based Precursor Inks. *Adv. Energy Mater*. 2021, 11, 2003460.
DOI: 10.1002/aenm.202003460

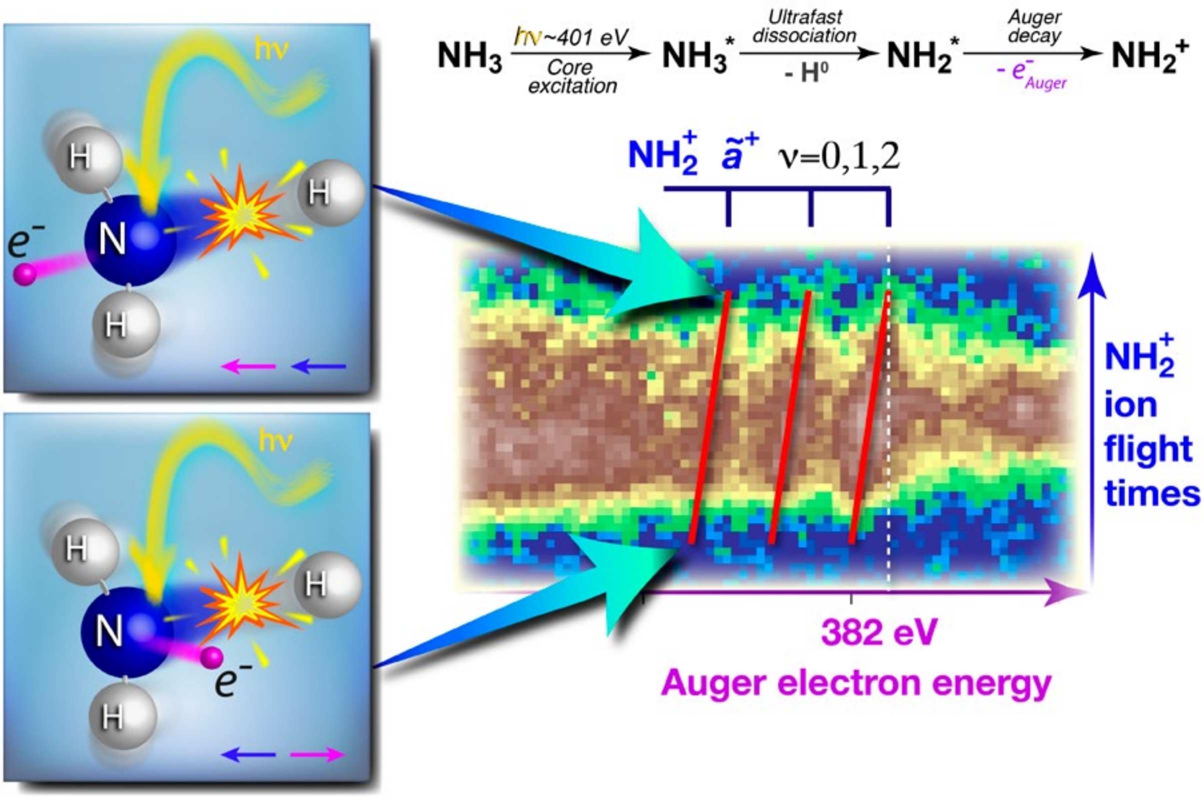
ENERGY AND FUELS

Molecular dynamics of the Auger Doppler effect

An international research group investigated the phenomenon of ultrafast dissociation with high-resolution coincidence spectroscopy using a high-energy high-resolution Gas-Phase End Station (GPES) setup at MAX IV's FinEstBeAMS beamline. The so-called Auger-Doppler effect was observed for the first time for the molecular fragment, when photon excitation of the N 1s core electron in the ammonia molecule creates an unstable core–hole state with a lifetime of only approximately five femtoseconds. Notably, scientists were able to characterize for the first time the redistribution of available energy after the Auger decay to excitations of the internal degrees of freedom–vibrations and rotations–in the molecular fragment. The work demonstrates the power of the high-resolution Auger electron–ion momenta imaging technique for future studies on the partitioning of excess energy between internal degrees of freedom in dissociating molecular fragments. The GPES setup combined with the state-of-the-art coincidence measurements revealed information otherwise hidden and undetectable in single-channel electron spectroscopy.

Ref:

O. Travnikova et al, Ultrafast dissociation of ammonia: Auger Doppler effect and redistribution of the internal energy. *Phys. Chem. Chem. Phys.*, 2022, 24, 5842-5854. DOI: 10.1039/D1CP05499F



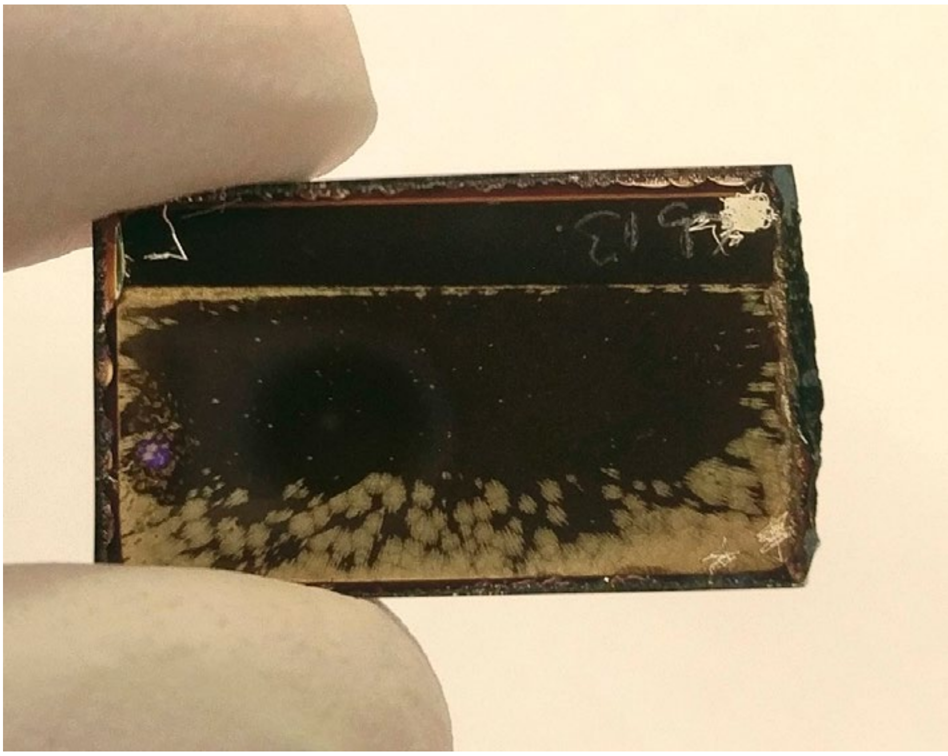
ENERGY AND FUELS

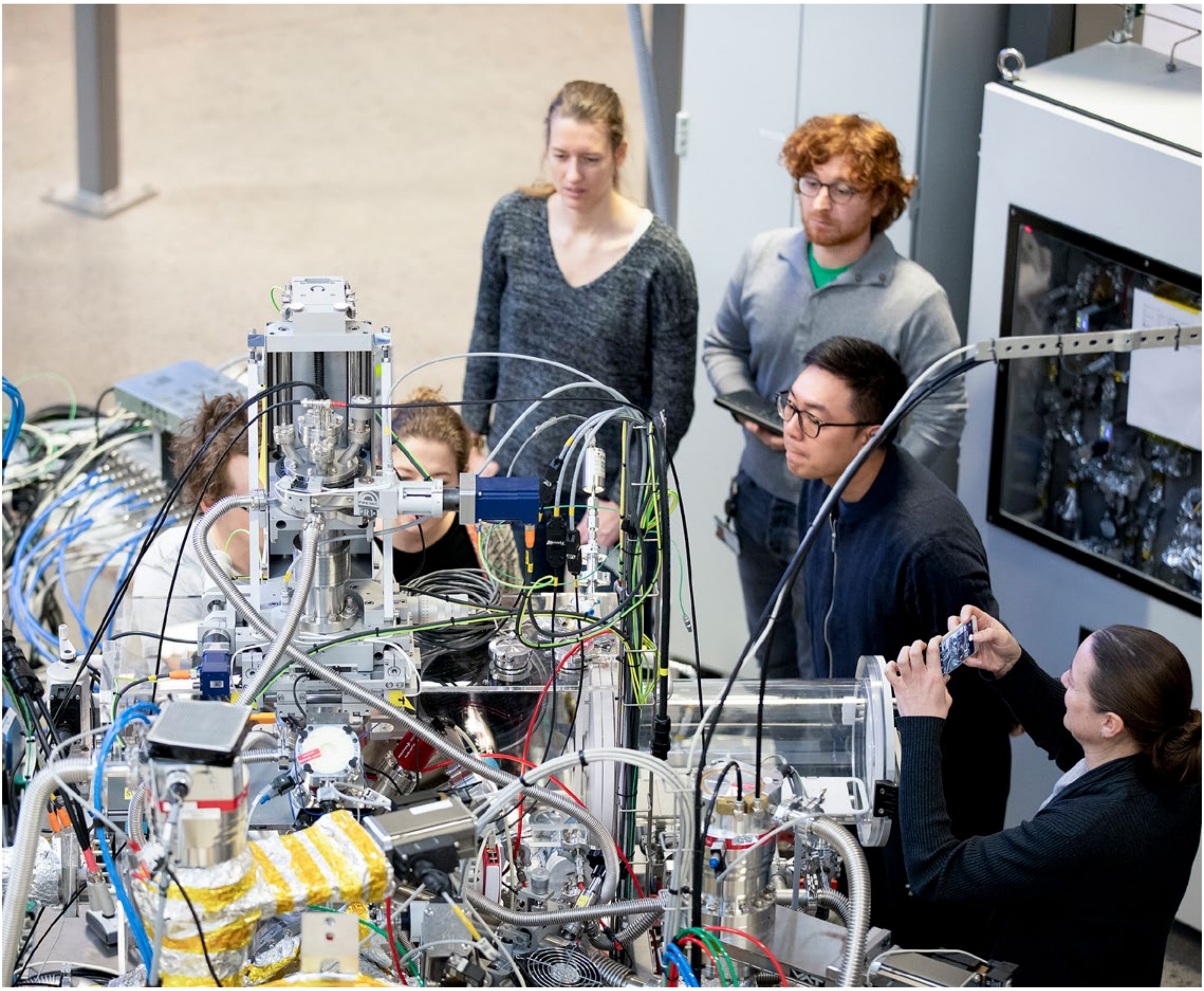
Degradation of copper electrodes in perovskites probed

Lead halide perovskite solar cells have reached a similar functional efficiency to crystalline silicon solar cells in recent years. Prohibitive costs for gold electrodes, the standard for research, and long-term stability issues with lower cost copper electrodes remain hurdles for advancement of perovskites application. Researchers at the Royal Institute of Technology (KTH) and Uppsala University investigated the degradation mechanism of copper electrodes in contact with lead halide perovskites. The chemical reactions between the perovskites and copper produced copper salt (CuI) and metallic lead. Additionally, an accelerated degradation of both the copper and perovskites occurred with oxygen and moisture exposure to form siidraite and copper-nitrogen complexes. The sample was characterised for atmospheric effects using Ambient Pressure Photoelectron Spectroscopy (APPES) at SPECIES beamline at MAX IV Laboratory. A firm understanding of the degradation mechanism could advance the development of stable electrodes alloys or barrier layers, and ultimately the broad commercialization of lead halide perovskite solar cells.

Ref:

S. Svanström et al. The Complex Degradation Mechanism of Copper Electrodes on Lead Halide Perovskites. *ACS Materials Au* 2022 *2* (3), 301-312 DOI: 10.1021/acsmaterialsau.1c00038





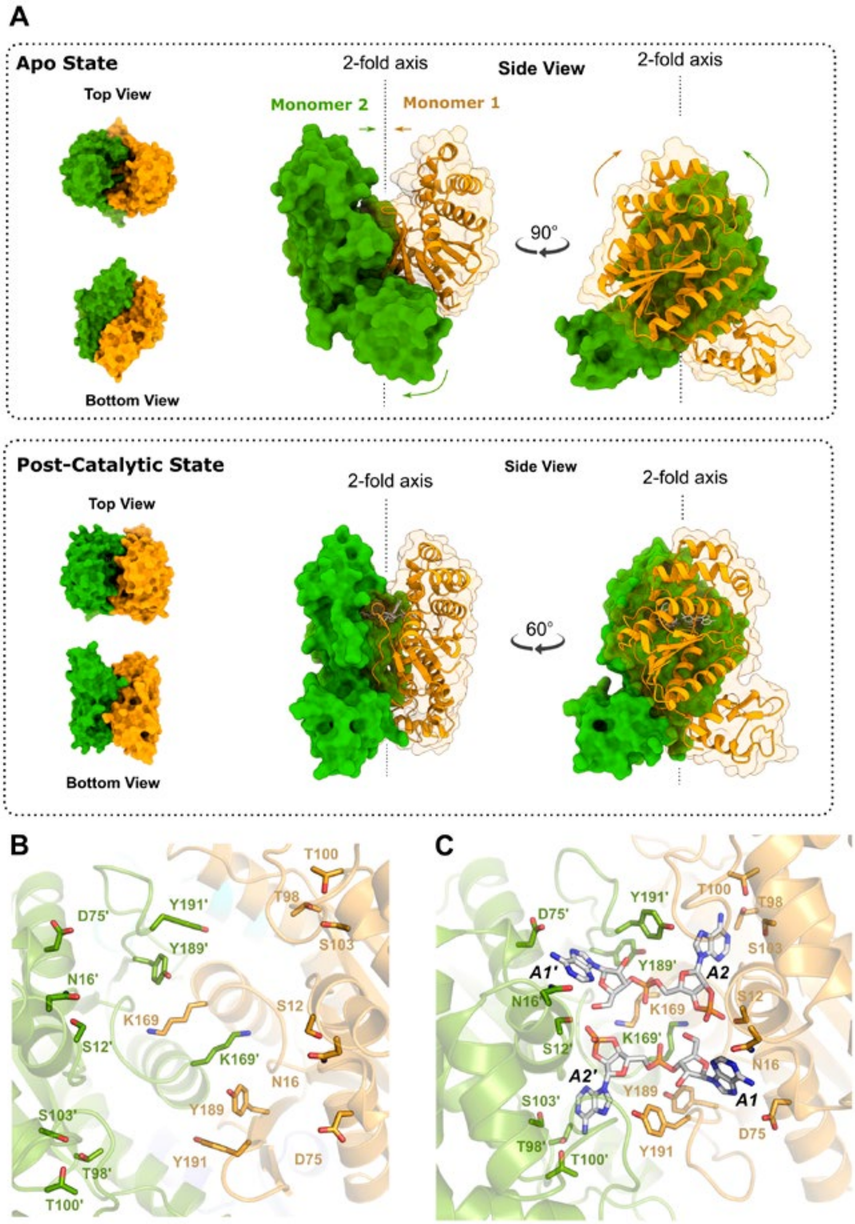
ENERGY AND FUELS

Modelling electrochemical potential for better Li-batteries

Many electrochemical processes necessary for battery function take place at the solid-liquid interfaces. Deciphering the influence of electrochemical potential differences during device operation is crucial for our understanding of these processes. A study from Uppsala University in Sweden and Karlsruhe Institute of Technology in Germany probed gold and copper model electrodes at MAX IV's HIPPIE beamline with Ambient Pressure Photoelectron Spectroscopy (APPES) during lithiation, otherwise known as charge transfer. The researchers followed changes in the electrochemical potential over these interfaces by measuring the kinetic energy shifts of the electrolyte levels, which could be correlated to the electrochemical reactions at the interfaces. The experimental setup thus allowed for an indirect probe of the electrode/electrolyte interfaces. The results further knowledge of electrochemical properties affecting chemical reactions in working batteries.

Ref:

I. Källquist et al. Potentials in Li-Ion Batteries Probed by Operando Ambient Pressure Photoelectron Spectroscopy *ACS Applied Materials & Interfaces* 2022 *14* (5), 6465-6475 DOI:10.1021/acsami.1c12465



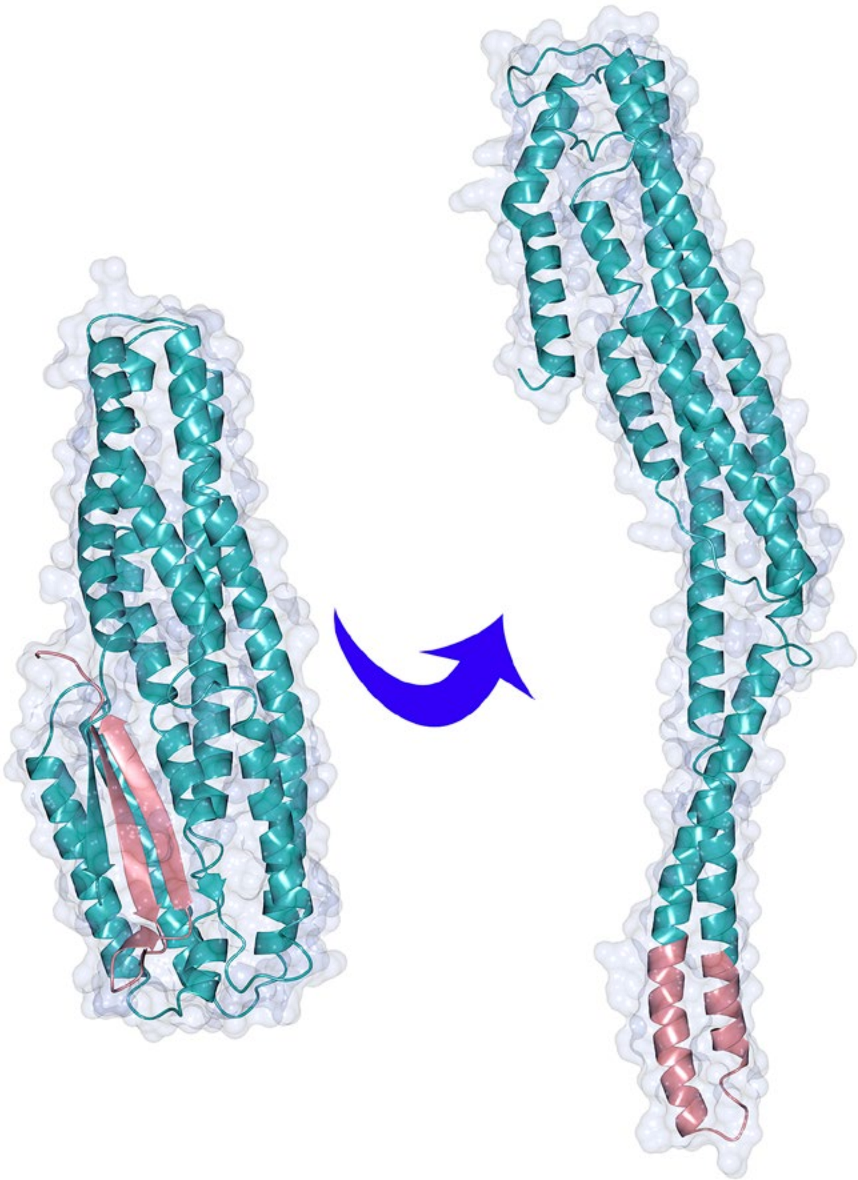
STRUCTURAL BIOLOGY

CRISPR-CAS mechanism described for RNA degradation off-switch

Scientists at the Novo Nordisk Foundation Center for Protein Research at the University of Copenhagen have illustrated for the first time the catalytic mechanism of a type III CRISPR-Cas stand-alone ring nuclease in atomic detail. Cyclic oligoadenylate molecules (cA_4) produced by CRISPR effector complexes, act as a secondary messenger to activate CRISPR ancillary nucleases which degrade foreign RNA. Indiscriminate RNA degradation can result in cell dormancy or death. To combat this, ring nucleases bind and degrade cA_4, disabling ancillary nucleases action and 'switching off' the cell's antiviral state. The degradation of cA_4 initiates a conformational change transmitting the signal from the CARF domains to the wHTH domains. Atomic structures of the *Sulfolobus islandicus* (*Sis*) ring nuclease were determined in part at BioMAX beamline at MAX IV. Knowledge of how bacterial cells defence systems work holds promise for finding novel strategies against one of society's current critical health challenges: antibiotic resistance.

Ref:

R. Molina et al. Structural basis of cyclic oligoadenylate degradation by ancillary Type III CRISPR-Cas ring nucleases. *Nucleic Acids Research* 49, 21 (2021). DOI: 10.1093/nar/gkab1130



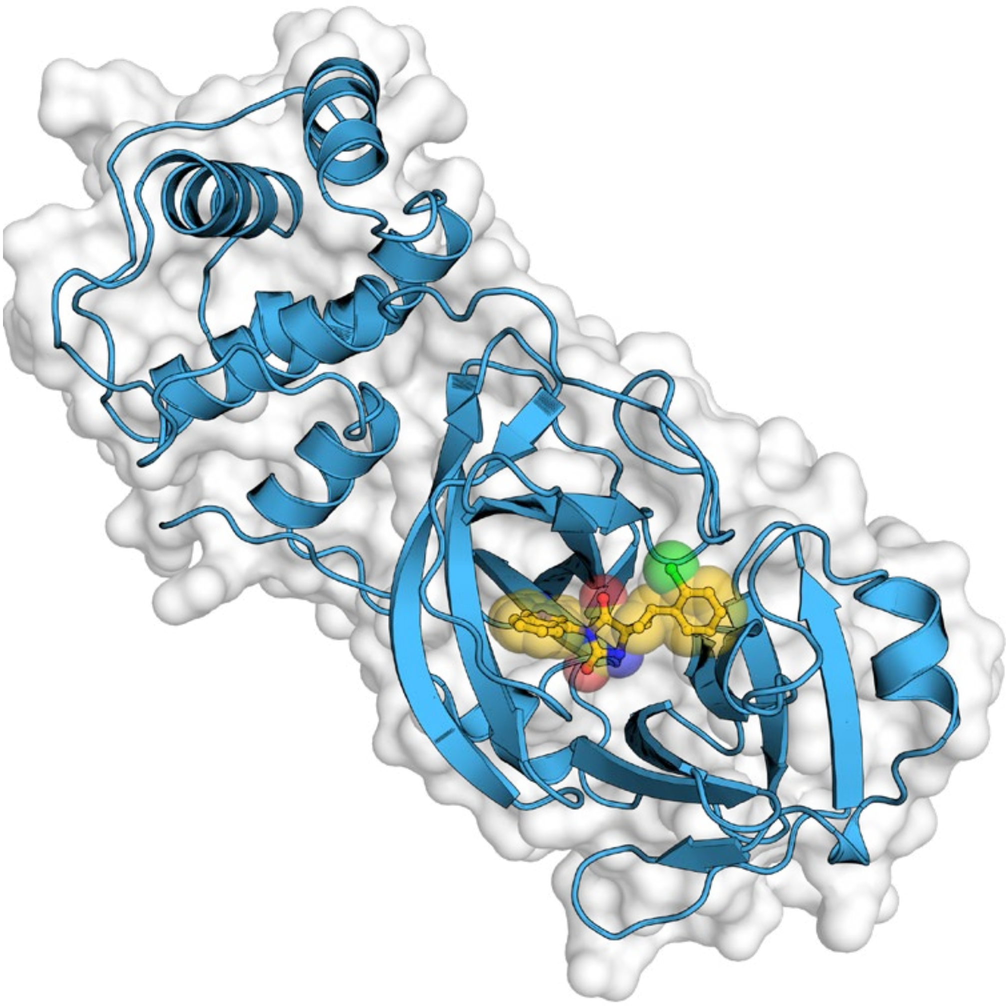
STRUCTURAL BIOLOGY

Flagellum aids toxin delivery of cholera bacteria

Researchers at Umeå University have discovered proteins, MakA, MakB and MakE, are secreted via the flagellum of cholera-causing bacteria, *Vibrio cholerae*. Together the proteins form a tripartite toxin that penetrates the membrane and causes lysis of the red blood cells. Diffraction data collected at MAX IV's BioMAX beamline was used to solve the structure of MakE. Together with the structures of MakA and MakB it was shown that hydrophobic residues are located on beta strands shielded from solvent by packing against a neighbouring helix. As a result, the group hypothesized that Mak proteins hide their hydrophobic parts until they encounter host cell membranes which triggers the formation of transmembrane helices and the subsequent formation of the tripartite toxin. The work illustrates a new creative bacterial infection mechanism. The knowledge from this study can in a longer perspective be explored for new diagnostics and therapeutic strategies for cholera disease.

Ref:

A. Nadeem et al, A tripartite cytolytic toxin formed by *Vibrio cholerae* proteins with flagellum-facilitated secretion. *Proc. Natl. Acad. Sci. U.S.A.* 118, (2021). DOI: 10.1073/pnas.2111418118



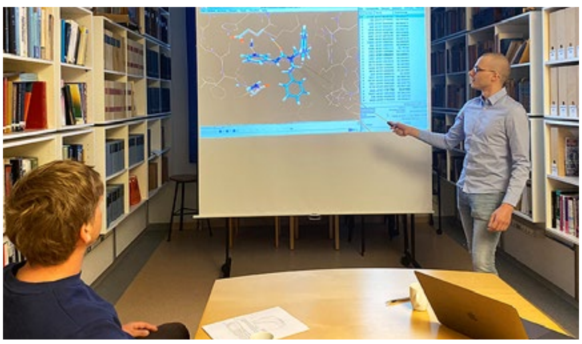
STRUCTURAL BIOLOGY

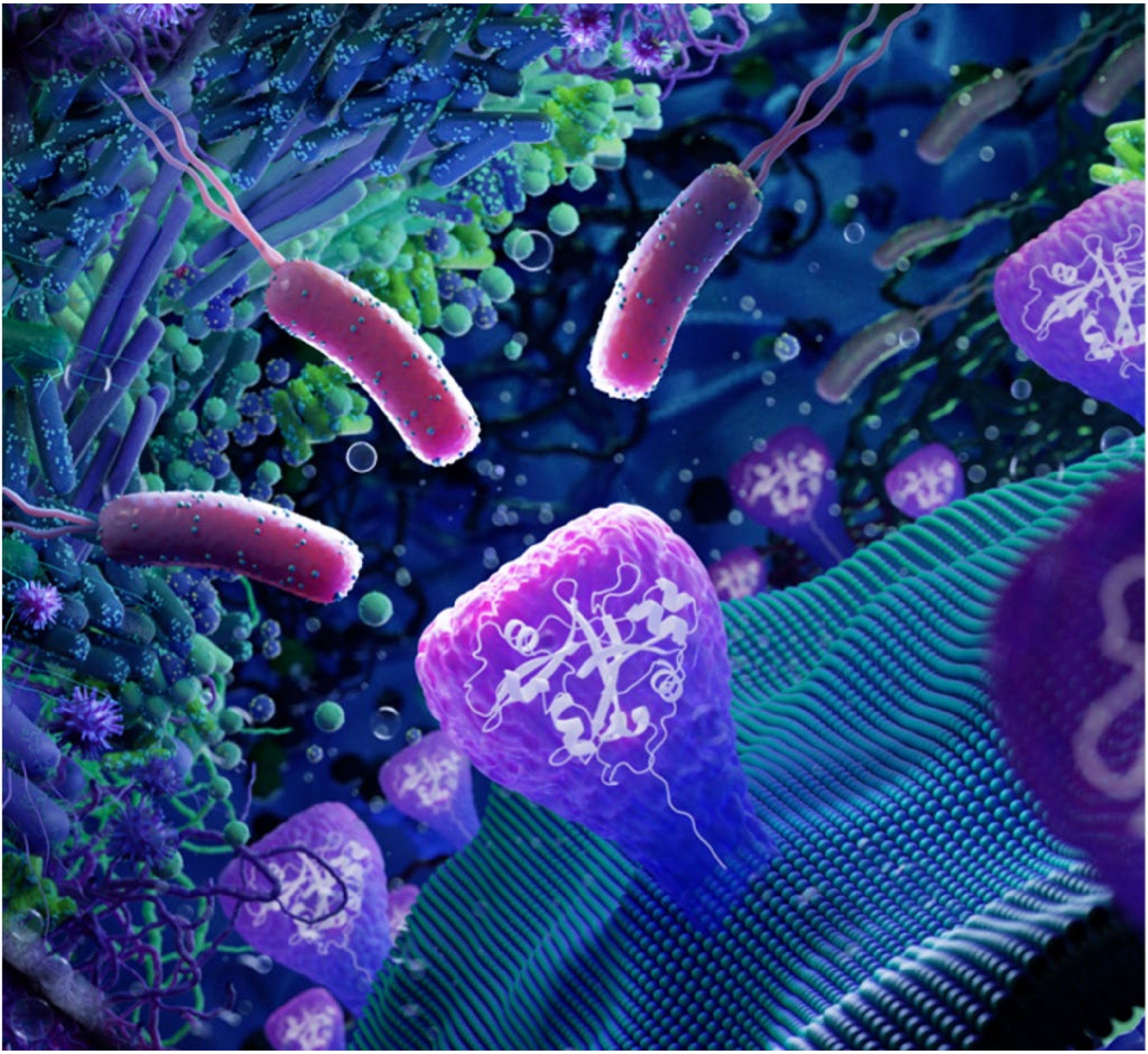
Potent inhibitor of SARS-CoV-2 replication designed

Scientists have uncovered an inhibitor of SARS-CoV-2 with a promising pharmacological profile and broad-spectrum antiviral effect against coronaviruses. A research team at Uppsala University performed virtual screenings of ultra-large compound libraries, with use of structure-based docking to the virus' main protease active site. Compounds predicted by the computational models were tested experimentally by the Drug Discovery and Development Platform at the Science for Life Laboratory (SciLifeLab). MAX IV's BioMAX beamline was used to determine crystal structures of the main protease in complex with identified inhibitors. Guided by the crystalline structures, a potent inhibitor was designed, which was determined to block the replication mechanism of SARS-CoV-2 in infected cells. The molecule is a promising candidate for the development of an antiviral drug treatment against Covid-19.

Ref:

A. Luttens et al. Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses. *Journal of the American Chemical Society* 2022 144 (7), 2905-2920. DOI: 10.1021/jacs.1c08402





STRUCTURAL BIOLOGY

How plants signal and control interactions with symbiotic bacteria

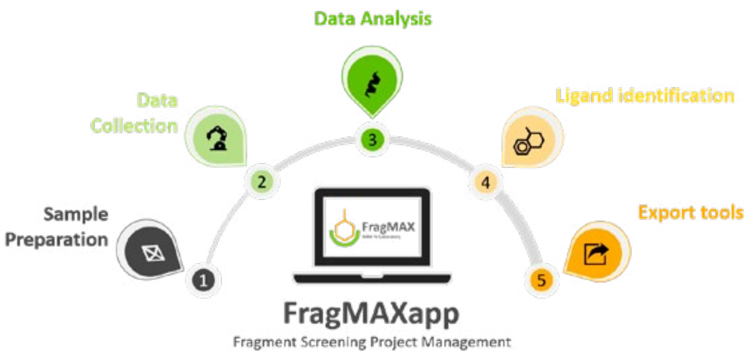
Plant cell surface receptors act as the communication connections for plants to engage with external microbes. The receptors bind carbohydrate signalling molecules, which enables the plant to recognize and allow interaction with symbiotic bacteria. With structural data from BioMAX beamline, an international research group has demonstrated that a class of lipochitooligosaccharide (LCO) receptors differentiate nitrogen-fixing bacterial symbionts with a kinetic proofreading mechanism that controls ligand receptor activation and signalling specificity. Further, they successfully engineered the binding site to support symbiotic functions—paving the way for future advances in receptor engineering in legumes and non-legume plants.

Ref:

K. Gysel et al. Kinetic proofreading of lipochito-oligosaccharides determines signal activation of symbiotic plant receptors. *Proceedings of the National Academy of Sciences*. 118.e2111031118. DOI: 10.1073/pnas.2111031118

STRUCTURAL BIOLOGY

FragMAXapp for large-scale data processing



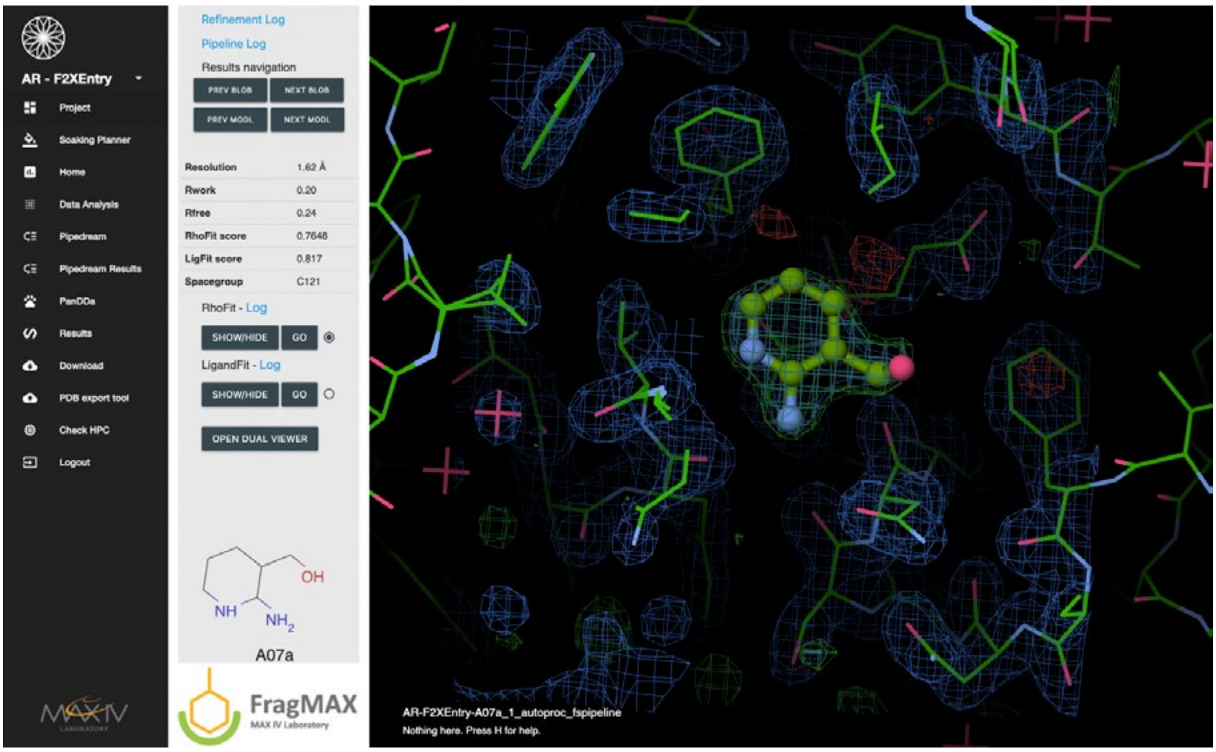
A joint team from MAX IV, SARomics Biostructures, Astra Zeneca, and LP3 of Lund University developed FragMAXapp, an integrated project management and analysis platform for large-scale diffraction data processing to support crystallographic fragment screening (CSF) experiments – a method to find starting points for drug development.

Through FragMAX web app, users can conveniently process and analyse their experiments from their home laboratory after the experiment. The web app facilitates data processing, structure refinement, automated ligand fitting, multi dataset analysis, and immediate 3D data visualization of data collected at the BioMAX beamline. The application is also accessible to all MX user at MAX IV Laboratory. It takes advantage of the MAX IV computer cluster and can simultaneously process hundreds of datasets, whereas traditional data processing suites allow only serial data analysis.

The FragMAX team is currently working with the European Protein Data Bank (PDBe) and other fragment screening centers to develop standardized data exchange formats to facilitate rapid data deposition and annotation. Moreover, the application has sparked interests from other synchrotrons and discussions about deploying it outside MAX IV is currently being discussed.

Publication

Lima, G. M. A.,et. al. FragMAXapp: crystallographic fragment-screening data-analysis and project-management system. (2021). *Acta Cryst*. D77, 799-808. DOI: 10.1107/S2059798321003818



AdaptoCell for MAX IV Laboratory users

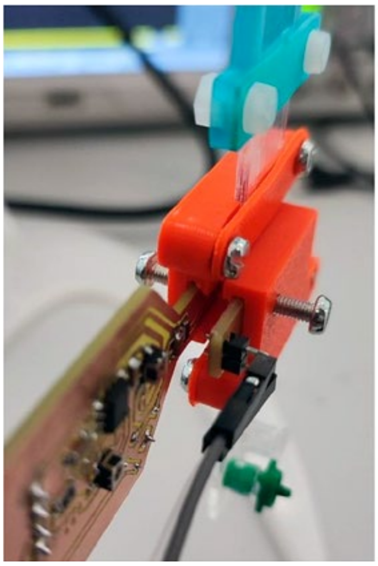
AdaptoCell is a user-friendly, adaptable microfluidic flow-cell platform at MAX IV Laboratory. Designed to facilitate user science and cater to user needs, it is a reconfigurable setup specifically developed for sample delivery at the following hard X-ray beamlines:

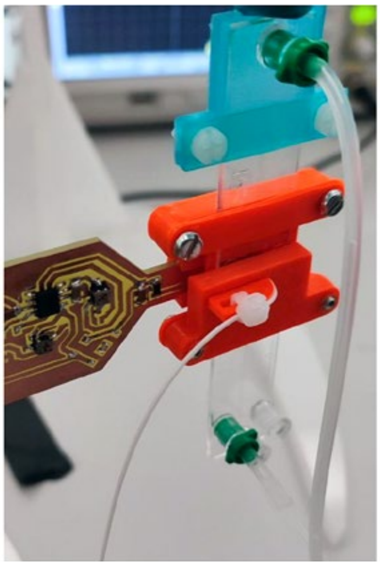
- Balder (X-ray absorption spectroscopy (XAS))
- CoSAXS (small-angle X-ray scattering (SAXS))
- BioMAX/MicroMAX (serial synchrotron crystallography (SSX))

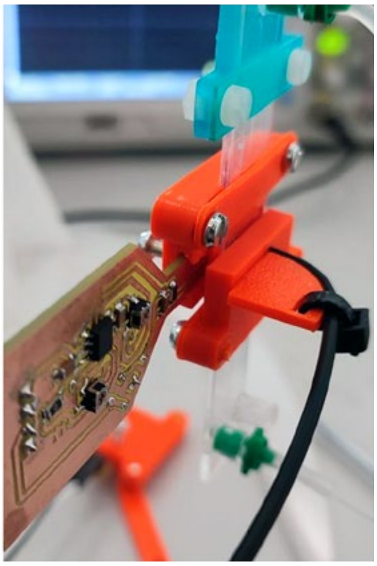
The beamline integrated systems allow for mixing (protein) solutions and excipients, temperature control of the flowed sample or hydrodynamic flow focussing samples for improved signal-to-noise ratios. The devices have been specifically designed with materials, device holders and logistic setups to ensure maximum hard X-ray compatibility.

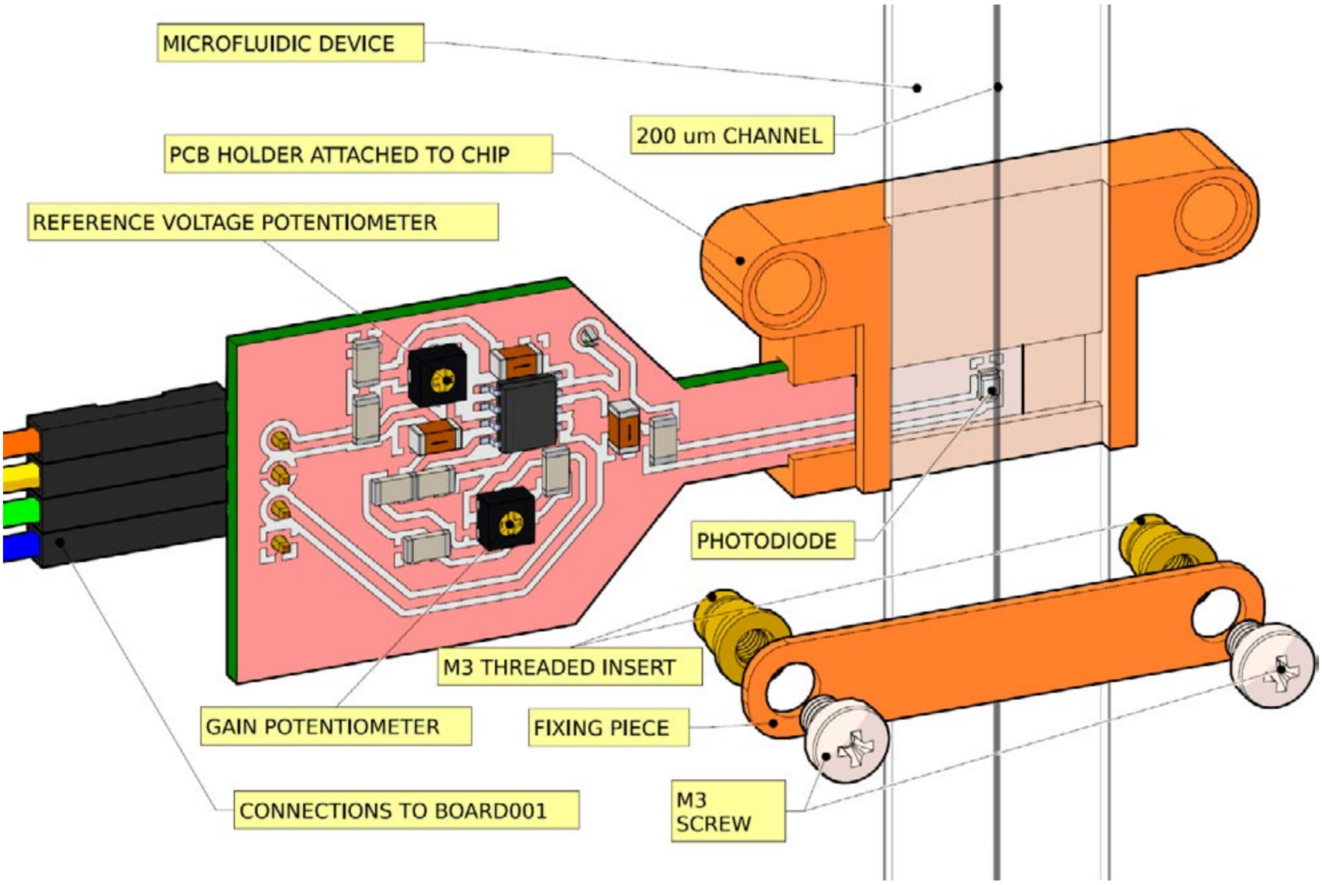
The initial target groups for AdaptoCell were those using XAS, SAXS and Macromolecular Crystallography (MX) for biological macromolecule investigation. Past research with these techniques has resulted in a plethora of unique and fundamental insights into life science. Although of extremely high importance to the area, the majority of previous studies have been performed with single sample sources without time-dependent mechanisms (such as response to introduced stimuli) and at biological non-functional temperatures (BNFT) (i.e., cryogenic or freezing temperatures).

These restrictions on the sample state and the information gathered from beamtime at synchrotrons often result when working with biological samples using high flux, intense synchrotron X-ray sources. Namely, sample damage from X-rays, difficulty introducing stimuli and 'black-box' methods of measurement (i.e., a sample is placed and measured with no data on the state or situation of the sample beyond the direct X-ray measurement). It has become increasingly apparent that many biological functions and structural changes/exchanges these measurement techniques seek to elucidate do not occur at very low temperatures and/or without stimuli – biology is warm and time-dependent.









AdaptoCell is user-friendly and enables the relatively straightforward application of XAS, SAXS and MX to time-resolved room temperature studies for the industrial and academic communities. From its inception, the core goal of the AdaptoCell project has been to create a common microfluidic architecture for the application of multiple analysis techniques at multiple beamlines at MAX IV Laboratory for the benefit of users.

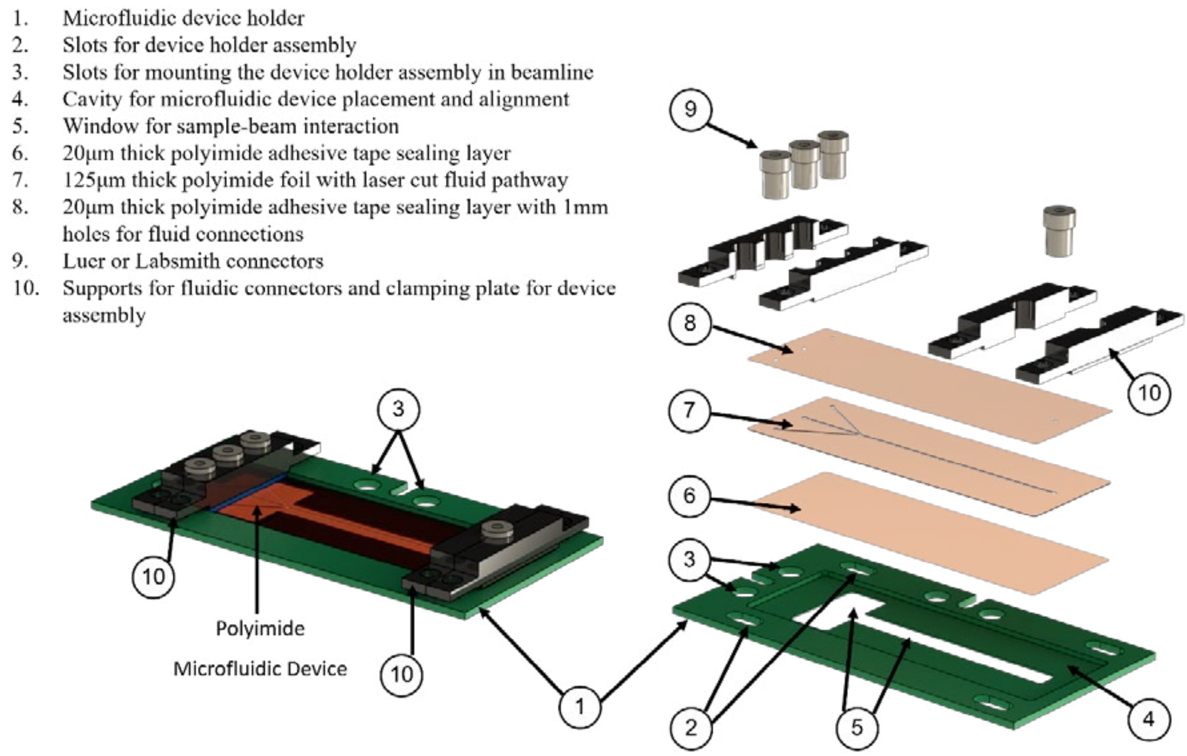
Adapted and commercial devices

Depending on the experimental requirements, different devices and flow cell solutions are available to users. Both commercial polymer chips (from Microfluidic ChipShop) and adapted custom-made devices, produced in collaboration with SciLifeLab Customized Microfluidics (Uppsala University), are available. The commercial polymer chips are injection-moulded in COC (cyclic olefin copolymer) and sealed with COC foil (140 µm thickness) which also works as the X-ray window. The chips show excellent X-ray properties and are available in different designs, e.g., straight channels, cross-junctions, droplet generators and mixing devices.

Various microfabrication techniques give one the flexibility to adapt chip design to the particular needs of a beamline user. In a recent publication, our team used a microfluidic device made of glass and silicon that could withstand high-energy X-ray beams and transport harsh solvent samples, such as lead solutions (Raj et al. 2021). For a different water-based application with proteins, a full polyimide chip was developed where laser cutting was employed to trim the fluidic channels. Hydrodynamic flow focussing can be applied in the microfluidic chip to avoid edge effects from the chip as well as reducing the sample volume consumption rate.

Off (beam)line station

In addition to the setup available at the beamlines, the AdaptoCell platform includes the development of an offline “twin” available at the MAX IV Biolab, a biological support lab located near the beamline stations. This offline setup allows the feasibility, experimentation and tuning of user-specific samples and requirements without the interference of awarded X-ray beamtime. The maximised system possibilities enable users to assess, configure and optimise the setup for



their specific needs prior to applying for or undertaking allocated beamtime.

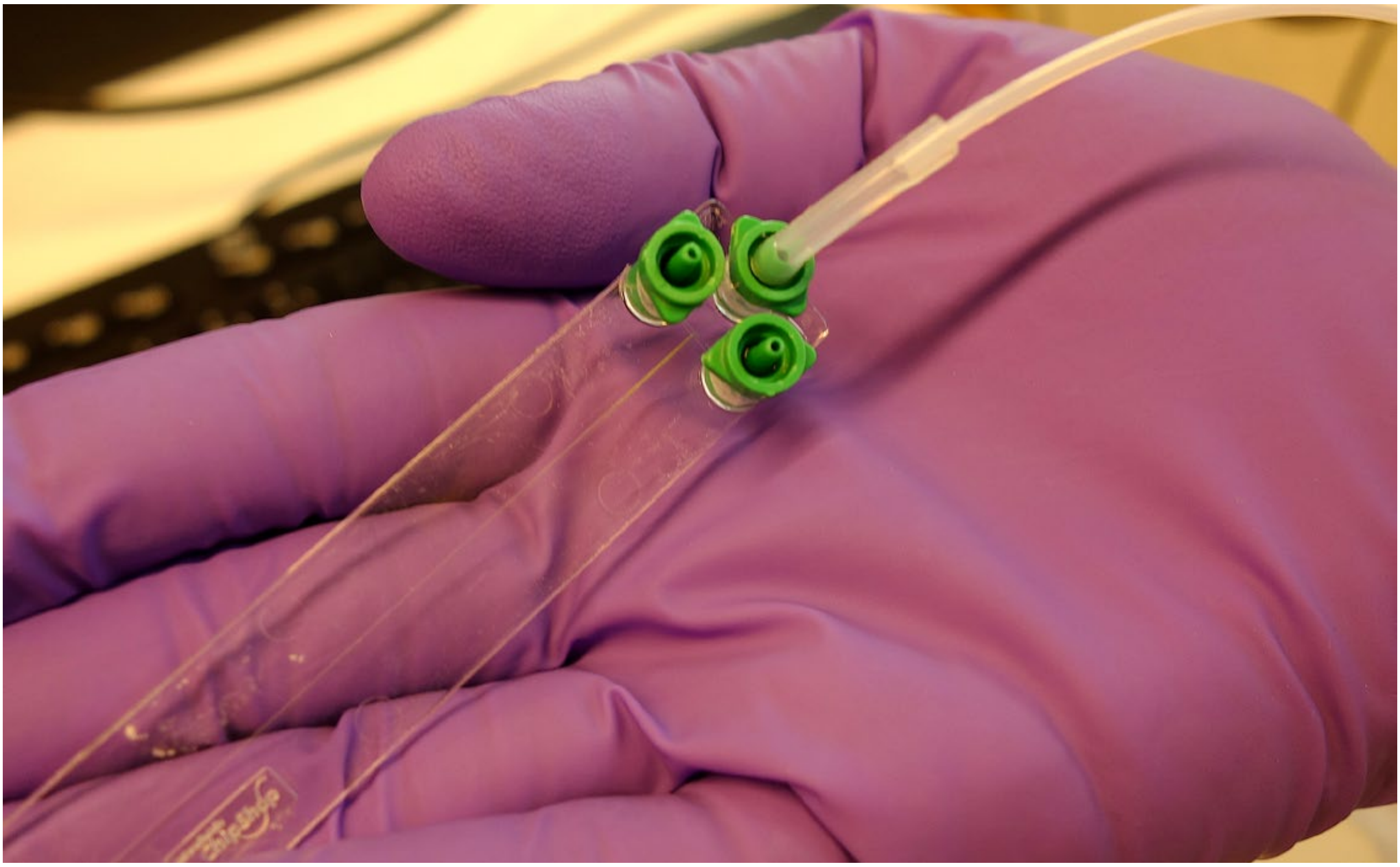
The offline station mimics the setup at the beamline, with a vertical chip mount on an optical microscope for visualisation of the micro channel. For high precision flow control, users can choose a pressure-driven flow system (ELVEFLOW) or syringe pumps (Cetoni). To ensure sample quality, users can check their samples before and after experiments by using dynamic light scattering, UV-vis (Nanodrop) and other protein assays available in the lab. The anaerobic chamber is crucial for producing and handling air sensitive samples and reduced states of redox active proteins, for example.

Beamline stations

Balder beamline provides X-ray absorption spectroscopy (XAS) in the medium to hard energy range, 4–40 keV. The beam is focused to 50 × 50 μm^2 and has a flux of 10^{12}–10^{13} photons /sec. It can be further reduced in size with a movable aperture down to 10 µm-range (with loss of flux) to match the sample flow width.

These are typical beam characteristics for the three hard X-ray beamlines and Balder was the first to be setup. AdaptoCell is particularly useful to investigate water-based liquid samples at ambient conditions, where the sample can be constantly refreshed to minimise the effect of radiation damage. The microfluidics device offers efficient delivery with decreased sample consumption and add-on functionalities. Balder has a pressure-driven flow control system integrated at the beamline and holders for both commercial and custom-made devices with a full range of translations in the beam. At Balder, AdaptoCell has, for instance, been used to investigate metalloproteins (heme) in solution as well as ink properties for photovoltaics.

The AdaptoCell platform is also integrated at **CoSAXS** beamline and has already been used by both academic and industrial users. At CoSAXS, commercial polymer chips are primarily used, while a specialised chip holder with temperature control and integrated heating is available for users to perform experiments at physiologically relevant temperatures. Examples of user applications include studies on the effect of shear stress on protein phase transition, observation of nanoparticle generation in a mixing chip, and study phase separation of intrinsically disordered proteins.



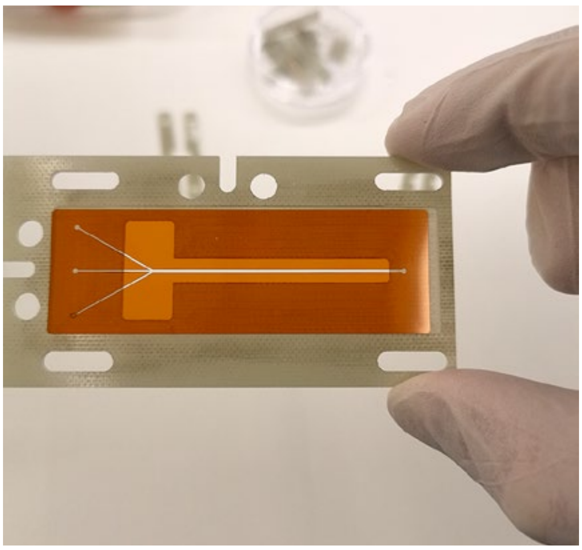
The third application of AdaptoCell devices is to flow microcrystals intended for synchrotron serial crystallography (SSX) with integrated crystal counting, à la lab-on-a-chip. This development is planned for the launch of the new **MicroMAX** beamline. Initial tests and development were performed at BioMAX and the partner lab at Halmstad University.

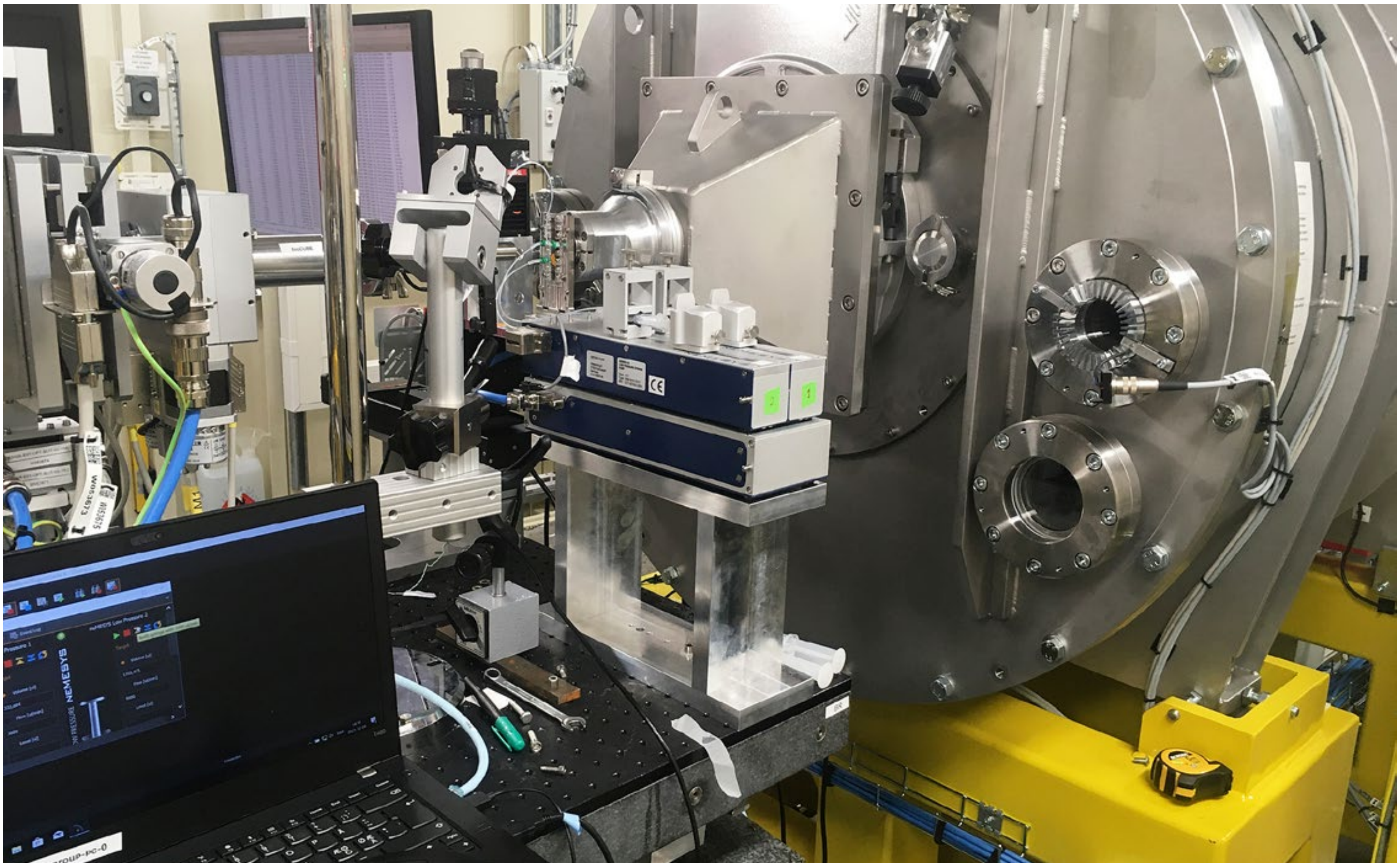
Lab-on-a-chip – beyond pure sample delivery

With the onboarding of crystal identification and integration of UV-Vis spectroscopy and device heating, AdaptoCell devices have moved beyond pure microfluidics and into the realm of lab-on-a-chip systems. The devices can provide additional data pertinent to the study technique employed. For example, the use of an attachable optical monitoring system allows for the detection of bubbles and potentially crystals in a crystal-containing fluid sample. This system is then connected to a micro-controller that provides a trigger signal for when unwanted/desired targets are detected, which can be used to synchronise with the SSX data collection. This could significantly increase the efficiency by which data is collected.

A second example is an integration of UV/Vis spectroscopy before and after the X-ray beam interaction that allows for additional *in-situ* data to be combined with X-ray study data to enhance knowledge about the target sample before and after X-ray beam interaction.

In addition to augmenting analysis, the multiple inlets of AdaptoCell devices allow for the controlled mixing of multiple solutions on board the device. With the fluidic flow control this mixing





can be carefully timed and the X-ray investigation technique synchronised with the mixing event and followed in time along the channel. This has important applications for the identification of kinetic and dynamic processes that occur, for example, the effect of pH titration with respect to protein conformations and enzyme catalysis.

AdaptoCell's lab-on-a-chip capabilities continue to develop, and the platform offers users more than just an advantageous method of sample handling and presentation—it offers potentially new insights to boost those of the beamline analysis techniques.

Future outlook

The AdaptoCell system is comprised of equipment as well as the know-how and experience of the lab scientist who aid users to deliver successful science. The AdaptoCell concept is inherently flexible and likely transferable to many of the beamlines and techniques at MAX IV Laboratory. As more researchers with a broader array of needs utilise the AdaptoCell setup, it will continue to evolve together with the user community to enable the study of samples in new levels of detail and environments.

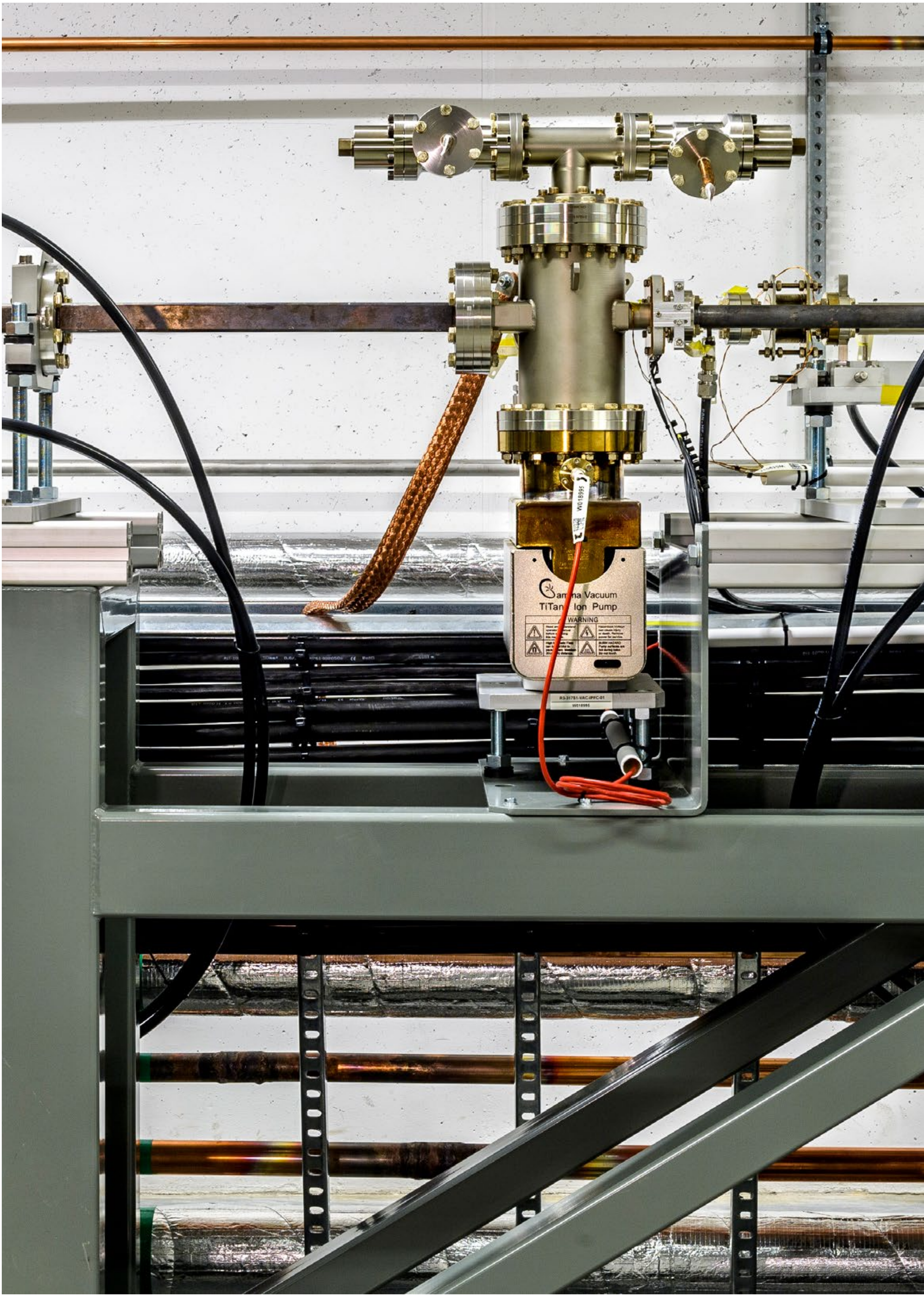
Present advances in the project equip the basic flow devices for lab-on-a-chip techniques which are user ready. In addition, new onboard stimulus techniques, such as light activation, are being developed for specific user needs. New vision-based analysis techniques are also currently being developed to improve the positioning possibility and timing synchronisation for microcrystal diffraction analysis.

Funding

The AdaptoCell project was fully funded by the Swedish Foundation for Strategic Research (SSF) (grant ITM-17-0375) for three years. This MAX IV-based project was established for users by the work of two postdocs and a team of five expert scientists at MAX IV, Uppsala University, and Halmstad University.

Publication

Raj PM et al "Fabrication and characterisation of a silicon-borosilicate glass microfluidic device for synchrotron-based hard X-ray spectroscopy studies" RSC Advances 2021. DOI: 10.1039/d1ra05270e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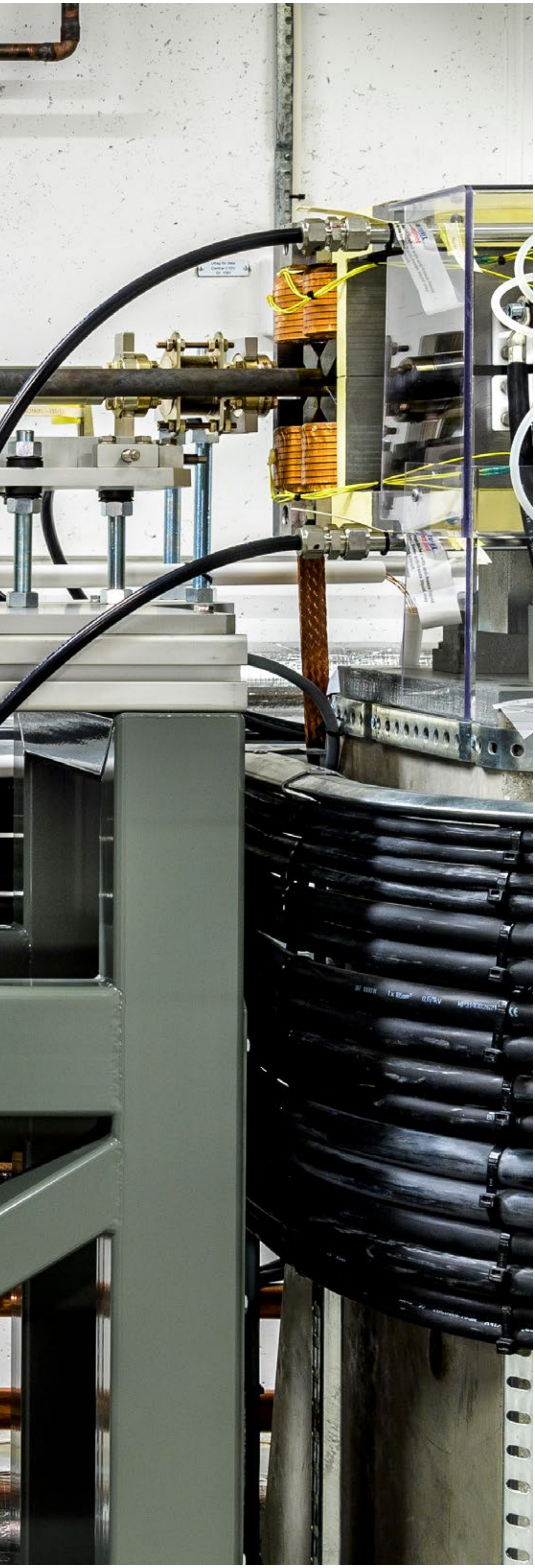

MAX IV Accelerators

Overview

2021 was marked by the significant impact of the COVID-19 pandemic on Accelerator Operations. The "warm shutdown" period implemented in the first few months of the year in response to the steep rise in infection rates in Skåne caused a reduction of the total number of scheduled beam hours. Moreover, delayed delivery of the insertion devices for the ForMAX and MicroMAX beamlines generated the need to re-schedule Accelerator Operations in the second half of the year, which further reduced the total number of hours delivered to the beamlines.

In contrast, and despite several failures in the injector RF stations mainly just before summer, accelerator uptime over the entire year either exceeded or came very close to our goals. In addition, the efforts of the project launched in 2020 to prevent short interruptions of the storage rings paid off beautifully, with clear improvement of the mean time between failures for the two storage rings.

The Conceptual Design Report (CDR) for a Soft X-ray Laser (SXL) driven by the MAX IV 3 GeV linac was completed in late February. The CDR was a joint effort by researchers and engineers at MAX IV Laboratory, Lund University, Lund Laser Centre, Stockholm University, Uppsala University, the Royal Institute of Technology, and the Stockholm-Uppsala FEL Centre. It received funding from the Knut and Alice Wallenberg Foundation. The design envisions the production of ultra-short pulses (i.e. down to a few femtoseconds (fs)) in the 1–5 nm wavelength region with full polarization control and two-pulse/two-colour capabilities. It will enable the development of future advanced capabilities such as Echo-Enabled Harmonic Generation, High Brightness SASE, and self-seeding. It will also provide experimental stations with an extensive range of pump lasers from IR to VUV. The SXL Scientific Advisory Committee reviewed the design and congratulated the SXL team for "a very well executed CDR" that "fulfils high international standards." The full CDR can be downloaded here, https://www.maxiv.lu.se/soft-X-ray-laser/ and a description of the Free-Electron Laser (FEL) can be found in.[1]

The 3 GeV ring vacuum system was the first implementation of a fully NEG-coated system in a synchrotron light source – Now, after several years of continuous and successful operation, a review published in April[2] describing the achieved performance and long-term behaviour confirms the expected outstanding results in terms of reliability and lifetime.

The stored beam current for routine delivery to the beamlines in the 3 GeV ring was raised from 250 mA to 300 mA in May. This was made possible by further optimization of settings for the main (100 MHz) and harmonic (300 MHz) RF cavity voltages as well as respective temperatures, which allow effective use of the available RF power.

The first attempts with experimental implementation of a reduced emittance optics in the 3 GeV ring were conducted, with a focus on improving the ability to detect the first pass of the injected beam. With tighter focussing, this optics reduces the stored beam emittance to approximately 270 pm rad, yet at the same time has a reduced dynamic aperture and larger sensitivity for errors. With nominal optics, the first few turns were ob-

1. W.Qin et al, *The FEL in the SXL project at MAX IV*, J. Synchrotron Rad. 28, 707 (2021).
2. M.Grabksi et al, Commissioning and operation status of the MAX IV 3 GeV storage ring vacuum system, J. Synchrotron Rad. (2021). 28 (2021).

tained without firing a single corrector. With the new optics, obtaining the first turn was significantly more time consuming and more sophisticated beam threading algorithms are expected to be required to achieve beam capture.

Developments for the 1.5 GeV ring focussed on improving the compensation of the disturbances caused by long-period elliptically polarizing undulators on the linear and non-linear beam optics. In 2021, various new knobs were made available for implementing such compensation – in particular, at the very end of the year, local compensation in the form of current strips attached to the vacuum chamber of the FinEst beam line undulator was installed. These are expected to be made operational in spring 2022. In addition, a project to provide the 1.5 GeV ring with the same Multipole Injection Kicker (MIK) system that has been in successful operation in the 3 GeV ring for several years was initiated in spring. The MIK aims at an improved transparency of the top-up injection and the first prototypes is slated for installation in mid-2022. Finally, work towards bringing pseudo-single-bunch capability into operation continued with further tests of the Transverse Resonant Island Buckets (TRIBs)[3] mode, which have been shown to operate successfully with up to 400 mA. This mode of operation follows pioneering work performed at the BESSY II synchrotron in Berlin and has the potential to allow simultaneous use of the storage ring by single and multi-bunch users.

Major development highlights for the linear accelerator include, observation of the first electrons from the 100 Hz RF gun (assembled to the Gun Test facility), the commissioning of a new gun laser system and a significant reduction of the electron beam size at the source point in the FemtoMAX undulators. Moreover, work by the newly created "Low-Jitter Task Force" showed the first results of a beam arrival monitor (BAM) developed in-house that demonstrated 50 fs rms time resolution.

The design of new high performance instruments using precision mechanics is another area of intense activity at MAX IV. Highlights in 2021 include a new detector table for the MicroMAX beamine, an aerodynamic lens system for the FinEst beamline, magnetic in-situ capabilities at the CoSAXS beamline, and KB mirror systems for the MicroMAX and SoftiMAX beamlines.

Finally, 2021 was a year where MAX IV as a whole, and the Accelerator Division in particular put much emphasis on planning for the next decades, through work on the MAX IV strategy plan. Many ongoing accelerator development activities described in the following pages are closely synergetic with those future plans aimed at providing ever brighter and more coherent beams to the Swedish and international user communities.

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3. D.K.Olsson et al, ***Studies on Transverse Resonance Island Buckets in third and fourth generation synchrotron light sources***, Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 1017, 165802 (2021).

Accelerator operations

During 2021, the COVID pandemic had its most significant effect on the daily operation of MAX IV, with a long period of so-called "warm shutdown" and very few on-site staff. During this time, however, the accelerators were kept in a quasi-delivery mode – RF on, beams stored, etc. – with the intention to prevent problems for restarting. This "warm" mode of operation implied that operations staff were required on-site during the entire period.

As the previous year, strong access restrictions to the control room constituted a major challenge to the Accelerator Operations team, and various digital tools developed since then have been put to intense use.

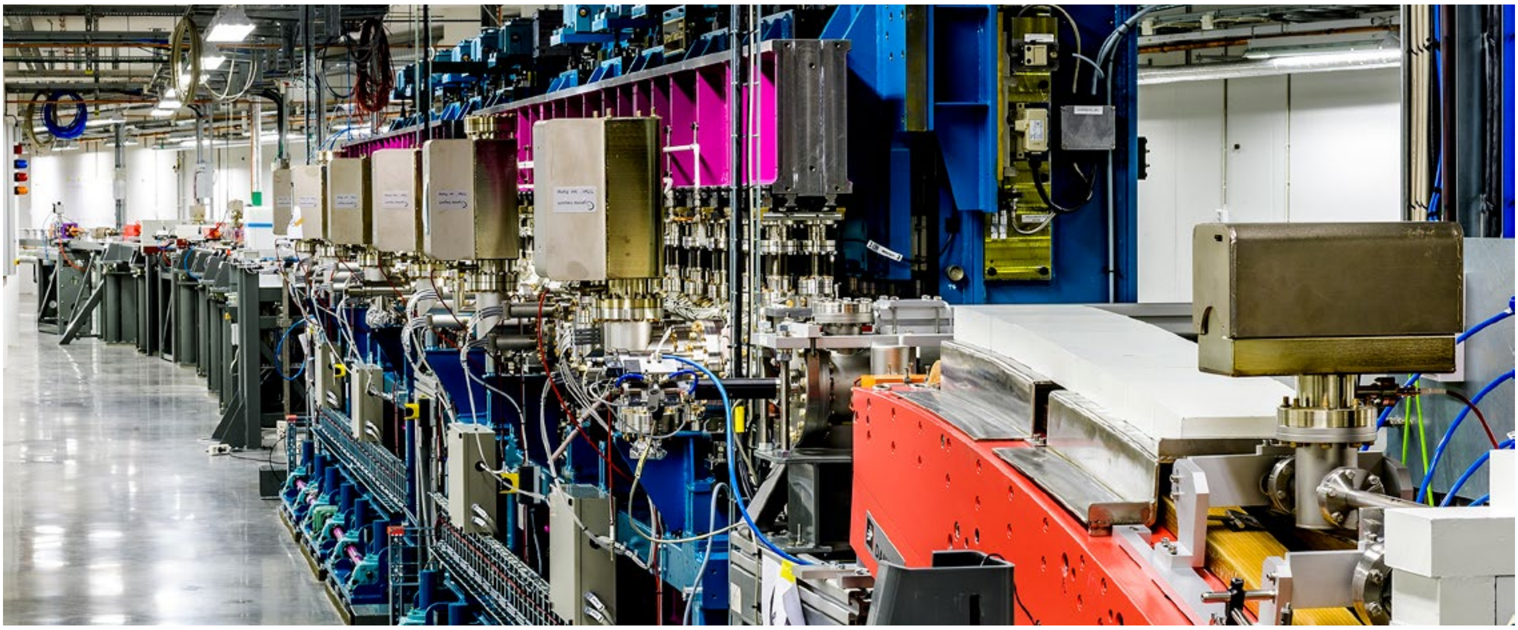
For 2021, the accelerator availability statistics are as follows:

Accelerator	Delivery (h)	Downtime (h)	Availability (%)	MTTR (h)	MTBF (h)
1.5 GeV Ring	3 888	108.2	97.22	2.16	77.8
3 GeV Ring	3 744	116.9	96.88	2.54	81.4
SPF	2 952	152.5	94.84	0.66	12.8

Two things are noteworthy. Firstly, despite a small number of long downtimes affecting all three accelerators (more details below), the availability of the 1.5 GeV ring exceeded the annual set goal whereas the availability for the 3 GeV ring and SPF came close to the goals of 97% and 95% respectively.

Moreover, it should be noted that the mean time between failure (MTBF) numbers for the two rings has climbed significantly from the numbers reported last year (56 hours for R1 and 40 hours for R3). As mentioned in the last report, a taskforce was set up to analyse the causes of the low MTBF, and deploy fixes, and it is noticeably very successful. The primary fix was to alter the way the automatic protection systems respond to certain events so the beam was not dumped unnecessarily. Doing this has eliminated a large class of downtimes, and so raised the MTBF by an impressive amount.

During June 2021, several failures of klystron/modulators in the linac occurred, which took away our ability to accelerate electrons to the required energy. Although there were only two events, each one resulted in more than a day of downtime for each of our accelerators, which affected the average availability. To lessen the chance of such events happening again, several actions have been taken. Our stock of spares has been increased, and more time has been devoted to conditioning of RF components. In addition, planning has started on a dedicated conditioning station to ensure that spare klystrons are ready to go with as little delay as possible.



3 GeV Ring

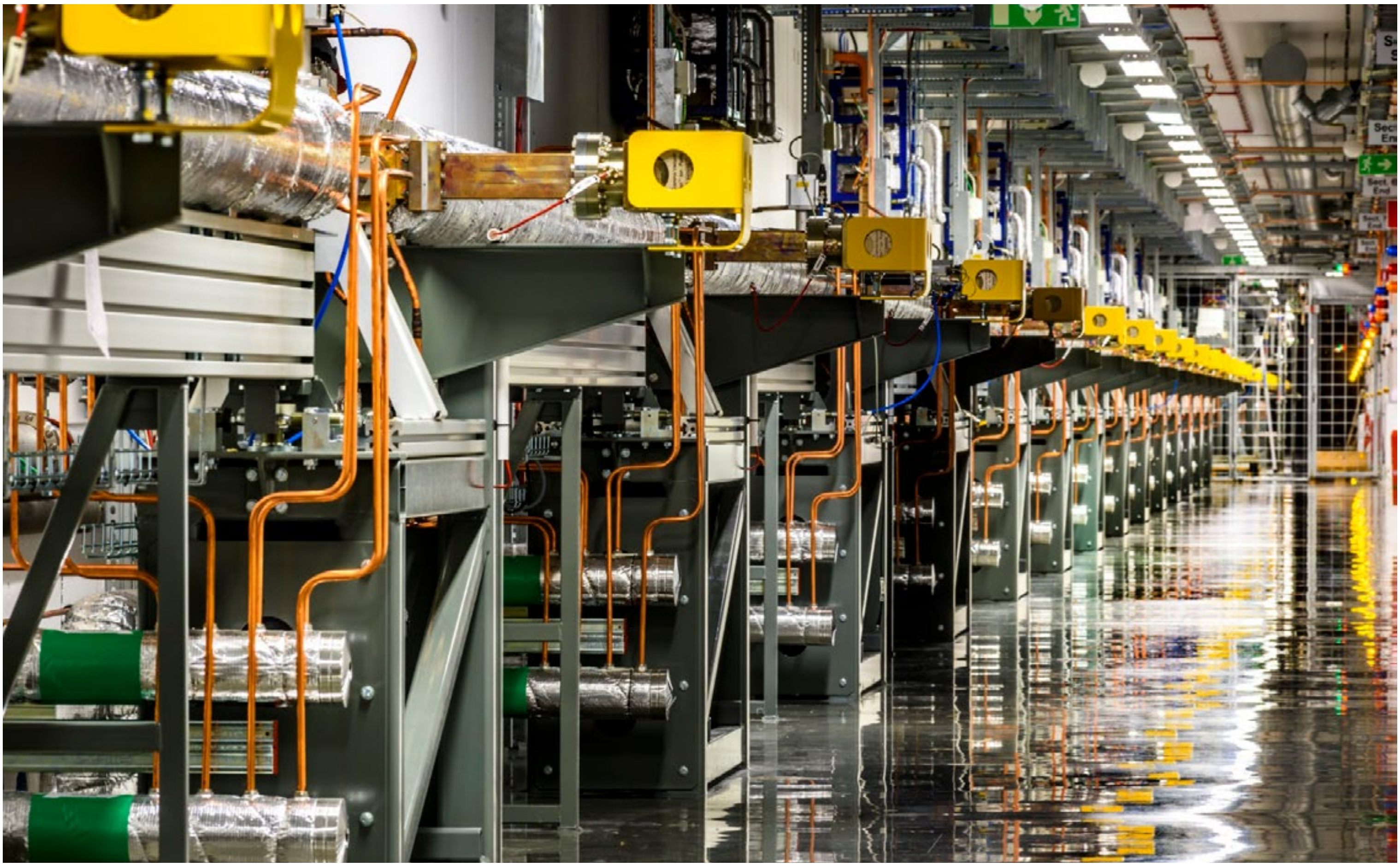
Increased delivery current

The stored beam current during delivery to beamlines in the 3 GeV ring was raised from 250 mA to 300 mA in May (Figure 1). This resulted from the application of the RCDS (Robust Conjugate Direction Search) algorithm that was used to find optimized settings for the main (100 MHz) and harmonic (300 MHz) RF cavity voltages as well as their temperatures. These procedures enabled the determination of settings for which the currently installed RF plant can provide, the necessary power to produce the required accelerating voltages, as well as fill up the passively operated harmonic cavities and replenish the energy the beam loses to synchrotron radiation emitted in bending magnets and insertion devices.

Figure 1: Screenshot of the MAX IV Status page on June 30th showing delivery at 300 mA top-up in the 3 GeV ring. It also shows the concurrent delivery of 400 mA in top-up for the 1.5 GeV ring and 10 Hz operation of SPF.

First tests of X Ray BPM-based orbit feedback

Blade-type X-ray beam position monitors are installed at all 3 GeV ring beamline frontends. For a few years these have provided a useful independent verification of the health of the beam orbit feedback systems, which are based on 200 electron beam position monitors located all around the ring. Despite the very high quality of the feedbacks, maintaining accurate positioning is particularly challenging in longer time scales. Studies were initiated in 2021 within the scope of the MAX IV Stability Task Force (STF) to verify which form of the X-ray beam position monitors could be made part of the feedback system and whether this indeed could lead to an improved stability as perceived by the beamlines. Figure 2 shows initial results that indicate sub-micron stability of the X-ray beam.



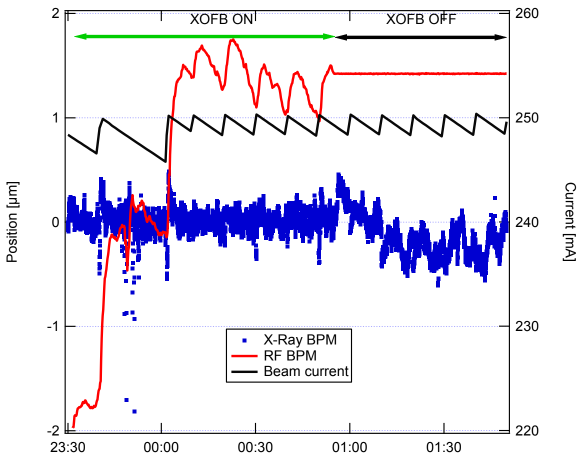


Figure 2: First test of orbit feedback based on X-ray beam position monitors at the BioMAX beamline.

Collective Effects Studies

Studies of various single and multi-bunch collective effects performed in 2021 included the modelling and beam-based characterization of Higher Order Modes in the main and harmonic cavities in the 3 GeV ring.[4] The ultimate goal of enhanced understanding of the driving forces of coupled bunch oscillations is to guarantee a high-quality photon beam. The narrow spectral speaks of high harmonics of short period undulators are particularly sensitive to the electron beam phase space dimensions and constitute an important characterization tool. Figure 3 shows the spectral flux measured at the 15th harmonic of the BioMAX beamline undulator at various beam currents, indicating the width of the peak is well maintained throughout the current range.

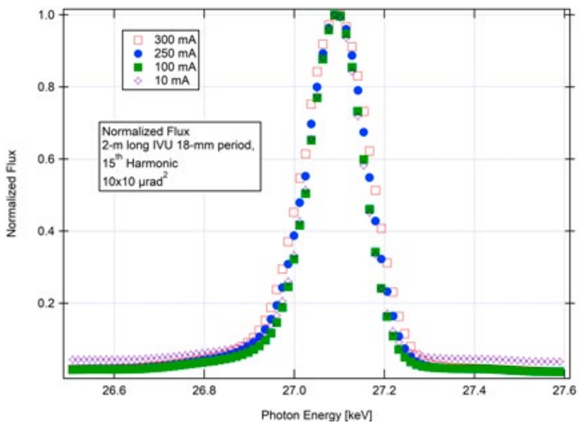


Figure 3: Spectral flux from the 15th harmonic of the BioMAX beamline undulator measured in a pin-hole geometry (narrow angular aperture) at various electron beam currents.

4. P.F.Tavares et al, *Beam-based characterization of higher-order mode driven coupled bunch instabilities in a fourth generation storage ring. Nuclear Inst. and Methods in Physics Research, A 1021 (2022) 165945*.

1.5 GeV ring

Compensation of perturbations produced by Insertion Devices

Today, the 1.5 GeV ring hosts 5 insertion devices (IDs) routinely producing soft X-rays. The majority of these devices are elliptically polarizing undulators, some of which have rather long periods and produce large perturbations on the stored beam. If uncompensated, these perturbations can be so intense as to compromise the beam lifetime and in extreme cases, even render injection impossible. Even though the simplest perturbations (on the electron beam closed orbit) can be effectively minimized with a combination of correctors built into the devices themselves and orbit feedback system using storage ring corrector magnets, perturbations to the optics, both linear and non-linear, can be considerably trickier to handle particularly for some polarization modes. In autumn 2021, the second phase of a five-phase project aimed at fully compensating the effects of insertion devices was completed. This allowed a considerable reduction of the effects of perturbations, in particular from the strongest IDs (FinEstBeAMS and BLOCH). Preparations for future phases include the installation of corrections to be implemented at the source of the perturbations, i.e. the IDs themselves.

Transparent top-up Injection

Following the successful operation of a multipole injection kicker (MIK) in the 3 GeV ring (Figure 4), a project initiated in 2021 to build, install, and commission a corresponding system for the 1.5 GeV ring. Initial efforts have concentrated on reviewing the dynamics of the injection process and assembling the engineering design of the various components for the kicker and its pulser. Even though initial design calculations for such a system were performed several years ago, a review was needed for several reasons – first the exact position of the MIK had to be changed to allow the old (dipole-kicker based) system to remain in place while the new one is commissioned. Second, as experience was gathered with the 3 GeV ring MIK, alternative options such as multi-turn injection became interesting as a mean of reducing the required pulser voltages.

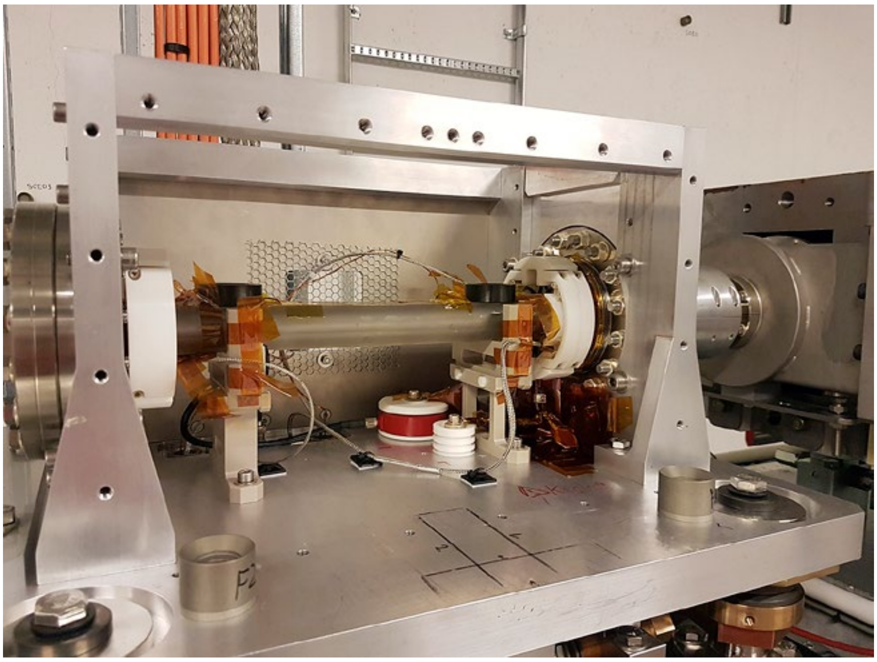


Figure 4: The Multipole Injection kicker installed in the 3 GeV ring. An identical component is planned for the 1.5 GeV ring.

Linear Accelerator

100 Hz Photocathode Gun

In late 2020, marked the successful implementation of operation of the linear accelerator at 10 Hz for delivery to the Short Pulse Facility as well as for injection into the storage rings. Focus now shifts to further increases towards the final goal of 100 Hz repetition rate. An important milestone in that project was achieved when the first electrons from the newly manufactured and mounted 100 Hz photocathode gun were observed on the 21st of October (Figure 5). The 100 Hz gun was installed in the Gun Test Facility earlier in the year and has undergone RF tests and conditioning. The first tests with beam were performed at low energy and produced 30 pC of laser produced electrons that reached approximately 2.5 MeV. Further conditioning and beam-based alignment are ongoing.

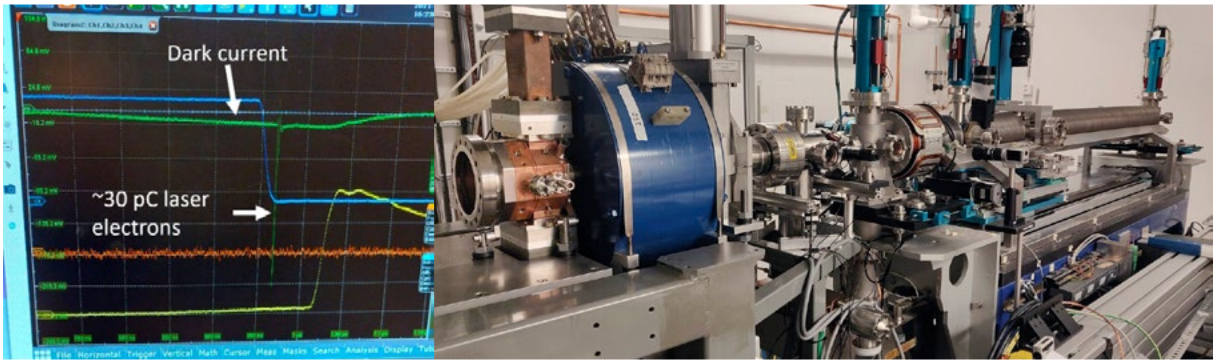


Figure 5: First electrons (left) produced from the 100 Hz photocathode gun installed in the Gun Test Facility (right).

Improved Emittance preservation along the linac

As a result of collective improvements, the emittance at the end of the main linac has been reduced by a factor of 6 (Figure 6). Where we priorly measured a projected emittance of 12 mm mrad or above, we can now routinely achieve 2 mm mrad. This considerable improvement was mainly achieved by the following developments that took place or produced results during the year:

- Separate power supplies for the dispersion quadrupoles and sextupoles in the bunch compressors.
- Alignment of magnets and linacs in the main linac[5] (done during 2020).
- Complement of Beam Position Monitors which produced a great improvement of beam trajectory control.

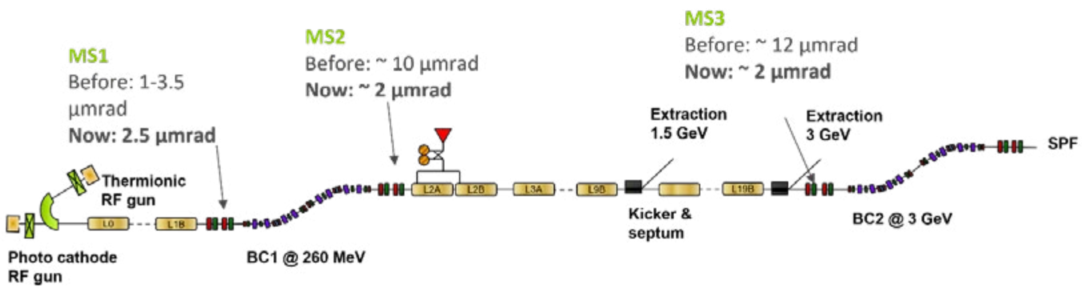


Figure 6: Preserving emittance though the main linac.

5. B. Afzali-Far et al, *Data analysis, spatial metrology network, and precision realignment of the entire MAX IV linear accelerator*, Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 1003, 165267 (2021).

Reduced transverse beam size for FemtoMAX

The transverse size of the X-ray pulse at the FemtoMAX beam line has been reduced from ~ 180 µm to ~ 70 µm (Figure 7). The primary reason for the substantial spot size improvement is the reduction in emittance mentioned above. We have also altered the position of electron beam focus along the undulator section. Focus was moved towards the end of the last undulator as it was reported from FemtoMAX that this is where most of the X-ray power emerges from.

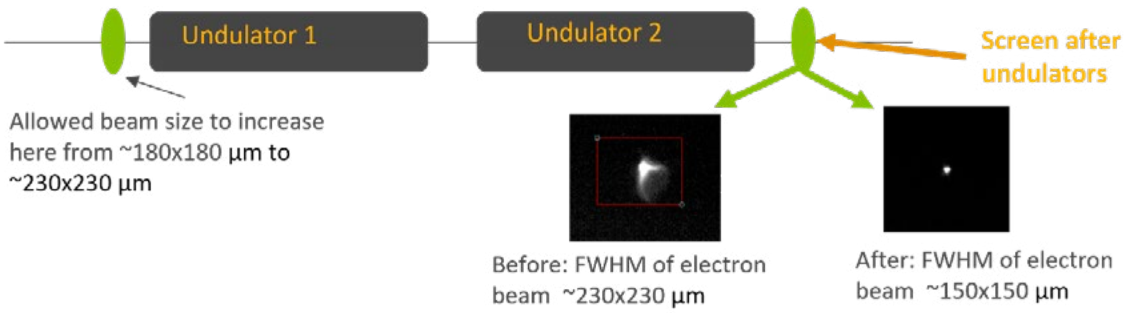


Figure 7: One of the methods to reduce beam size for FemtoMAX was to optimize the position of the electron beam waist through the undulator section. It was concluded that moving the focus closer to the end of the last undulator gave a smaller focus.

CTR longitudinal diagnostics tool

In collaboration with J. Wolfenden, T. Pacey, R. Fiorito and C. Welsch at the Cockcroft Institute (UK), a diagnostics tool for measuring electron bunch length was installed after BC2 (Figure 8). This tool uses coherent transition radiation (CTR) to provide information on the longitudinal properties of the bunch. The intensity of the CTR indicates the relative bunch length of the electron beam, while with further analysis, the hole in the centre of the CTR cone can give absolute numbers. Setup and tuning for FemtoMAX delivery now routinely use this longitudinal diagnostic tool to ensure short electron bunches.

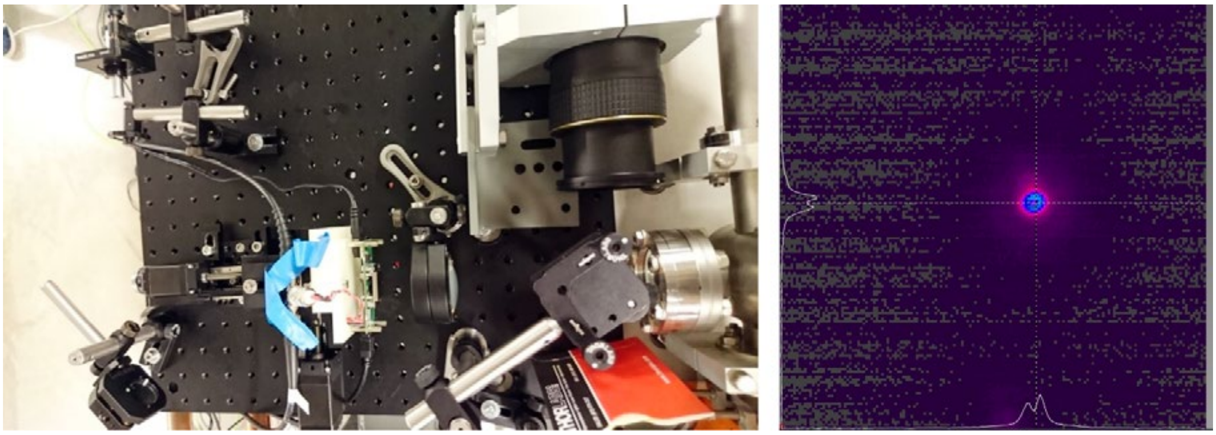


Figure 8: A relative bunch length measurement using CTR can now routinely predict maximum compression. It should also be able to give an absolute value after analysis.

Low Jitter Task Force

A Low Jitter Task Force (LJTF) was initiated in 2021, with the aim to provide the ultimate pulse-to-pulse repeatability. The focus of the task force is energy, arrival time, and bunch length stability, including the entire chain from gun laser, via the linear accelerator to X-ray pump laser probe in the beamline.

The accelerating fields in our linac structures are amplified in klystron tubes. We have demonstrated a working point, the "magic angle", where the energy jitter caused by phase and amplitude fluctuations from the klystrons cancel out (Figure 9).

The first tests where our electrical master RF oscillator is replaced by an optical master oscillator (OMO) have shown very promising results. Our OMO ensures improved arrival time of the gun laser relative the accelerating fields. The result was a significant reduction in energy and arrival time jitter of the electron beam (Figure 10).

To characterize improvements in the accelerator we are commissioning a beam arrival monitor (BAM). The BAM is based on a resonating cavity which is excited by the electron beam. By mixing the cavity field with a reference signal the arrival time phase is decoded on a carrier with significantly lower frequency, which is digitized and analysed. The BAM follows electron delays correctly and the resolution of the device is currently 50 fs RMS (Figure 11). Work is ongoing to improve the temporal resolution of the BAM.

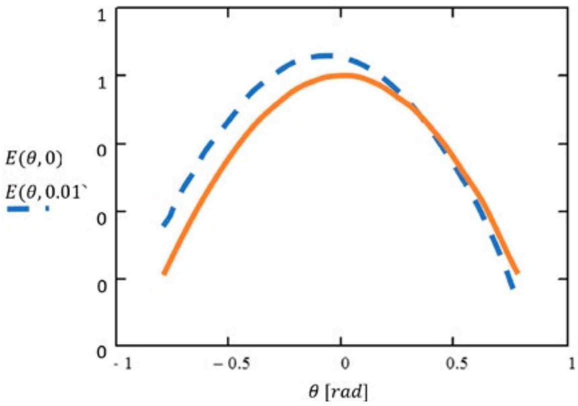


Figure 9: Energy gain in a linac structure as a function of accelerating phase. The nominal gain is plotted in solid red, while the dashed blue shows the gain after a correlated phase and amplitude change in the klystron tube. At the crossing point the klystron modulator voltage variations do not affect either energy gain or arrival time.

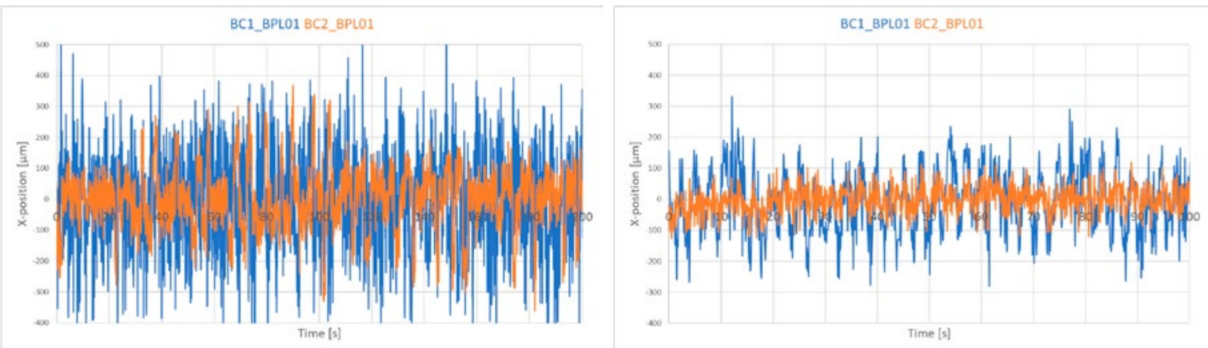


Figure 10: Transverse beam position variations as a function of time in the bunch compressors. The two beam position monitors (BPMs) are located at maximum dispersion. The position changes are thus proportional to energy deviation. The left plots show the performance achieved using the electrical RF oscillator and the right plots show the result of using the OMO. The RMS energy jitter was improved by a factor of two.

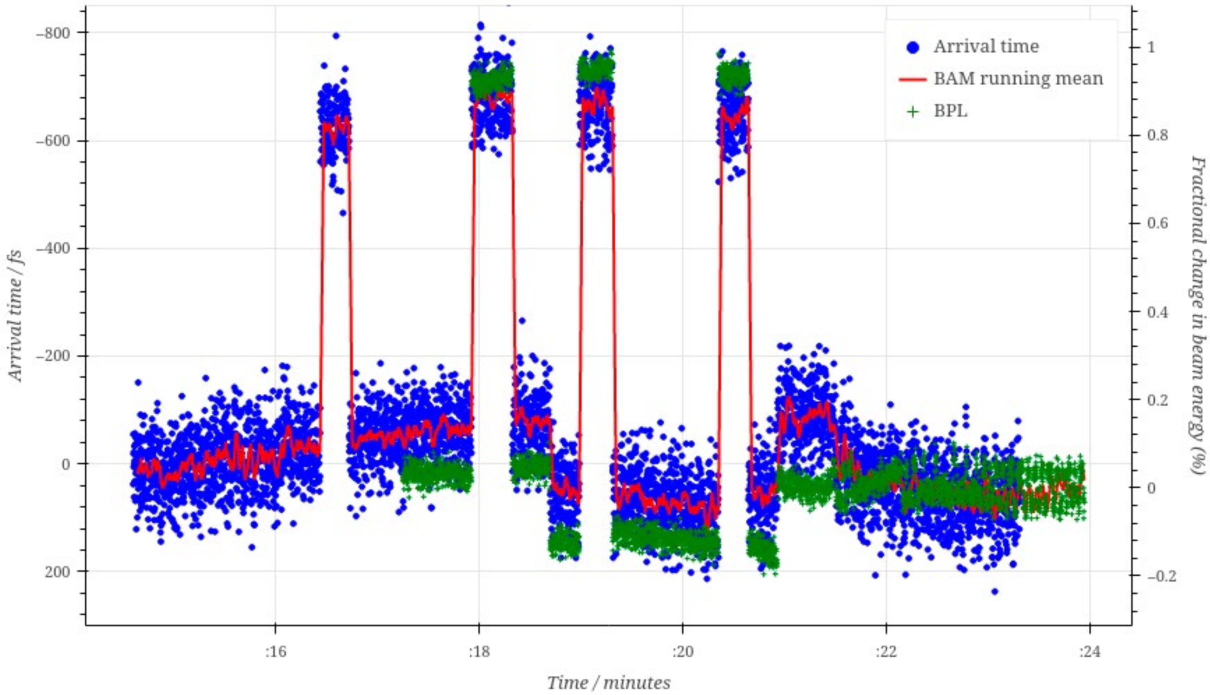


Figure 11: Beam arrival time and beam energy measurements. Blue is the arrival time whereas red is relative energy deviation energy deviation as determined by the change in beam position at a dispersive point of the lattice. The four large steps at around 17, 18, 19 and 21 minutes were generated on purpose by changing the beam energy at the entrance to the second bunch compressor. The fluctuations in-between those large changes include both actual arrival time jitter and drift as well as instrumental resolution and amount to 50 fs rms.

New Gun Laser System

In the last few years, the laser driving the photo cathode gun in the MAX IV linac has suffered from degradation of the oscillator crystal and required maintenance intervention every week. To ensure reliable and high-quality performance of the photo gun, a new laser was procured and taken into operation. The new laser can run for months without interventions and delivers 700 µJ at 263 nm. The old laser will now undergo considerable maintenance and will be able to function as a spare laser system for the photo gun as well as a driver for photocathode gun commissioning in the gun test facility.

Engineering Developments

Mechanical Design

The design of new high performance instruments using precision mechanics remains an area of active development at MAX IV with several highlights in 2021. One of them is the new MicroMAX Detector table (Figure 12), which will house two detectors and provide automated and rapid change between them.

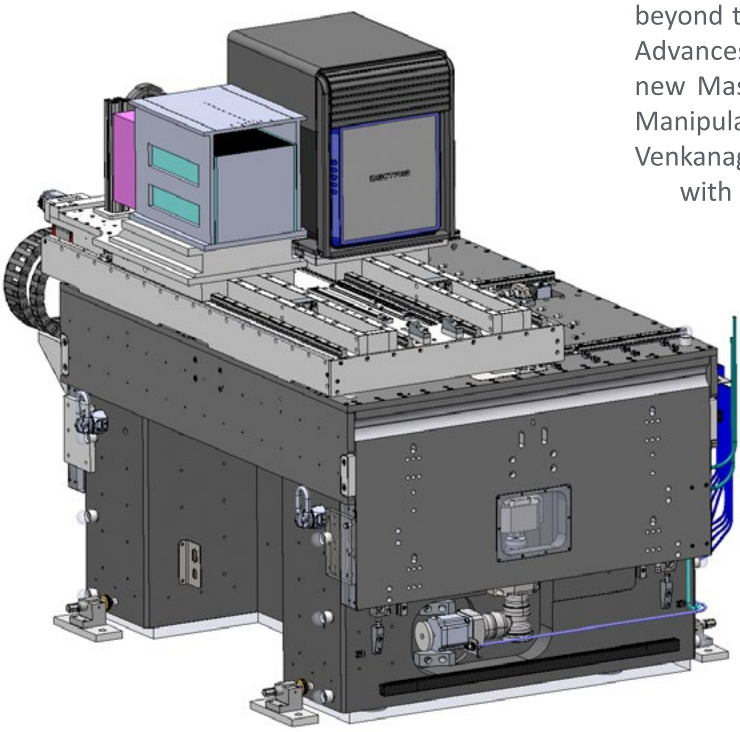


Figure 12: The new MicroMAX detector table.

Each detector will be centred to the X-ray beam and moved approximately between a closest position and 1m distance away. The main goal of the design is to achieve high resolution, accuracy, and stability during the horizontal, vertical, pitch and yaw movement. The design concept is based on a large granite base, front and back flexure plate attached to the upstream and downstream of the granite using high precision linear guides and connected by a horizontal plate. The pitch is achieved by a differential movement of the front and back plates. The change between the detectors is performed by conventional precision linear guides, meanwhile, the yaw is achieved by circular guides.

Project B.O.R.I.S. Bluelining Optimal Robotic Imprinting System

Initiated in 2020, the B.O.R.I.S project aims to develop an advanced robot that will bring the precision of equipment positioning to a level far beyond the one attainable by current methods. Advances made in 2021 include the start of a new Master thesis on "High Precision Robotic Manipulator for Blue-Lining at MAXIV" by Vinay Venkanagoud Patil as well as collaborative work with the SBUF (Svenska Byggbranschens Utvecklingsfond) development project by Peab, Cognibotics AB and LTH. For the latter, the "Buster" construction dog-robot visited MAX IV and tested the possibility of positioning by using our spatial metrology network. In addition, The Royal Physiographic Society of Lund has decided to award the grant: "Endowments for the Natural Sciences, Medicine and Technology – Technology" to partially fund the continuation of the project.

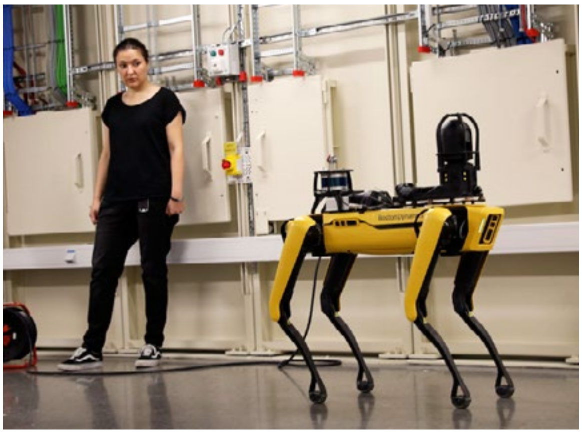
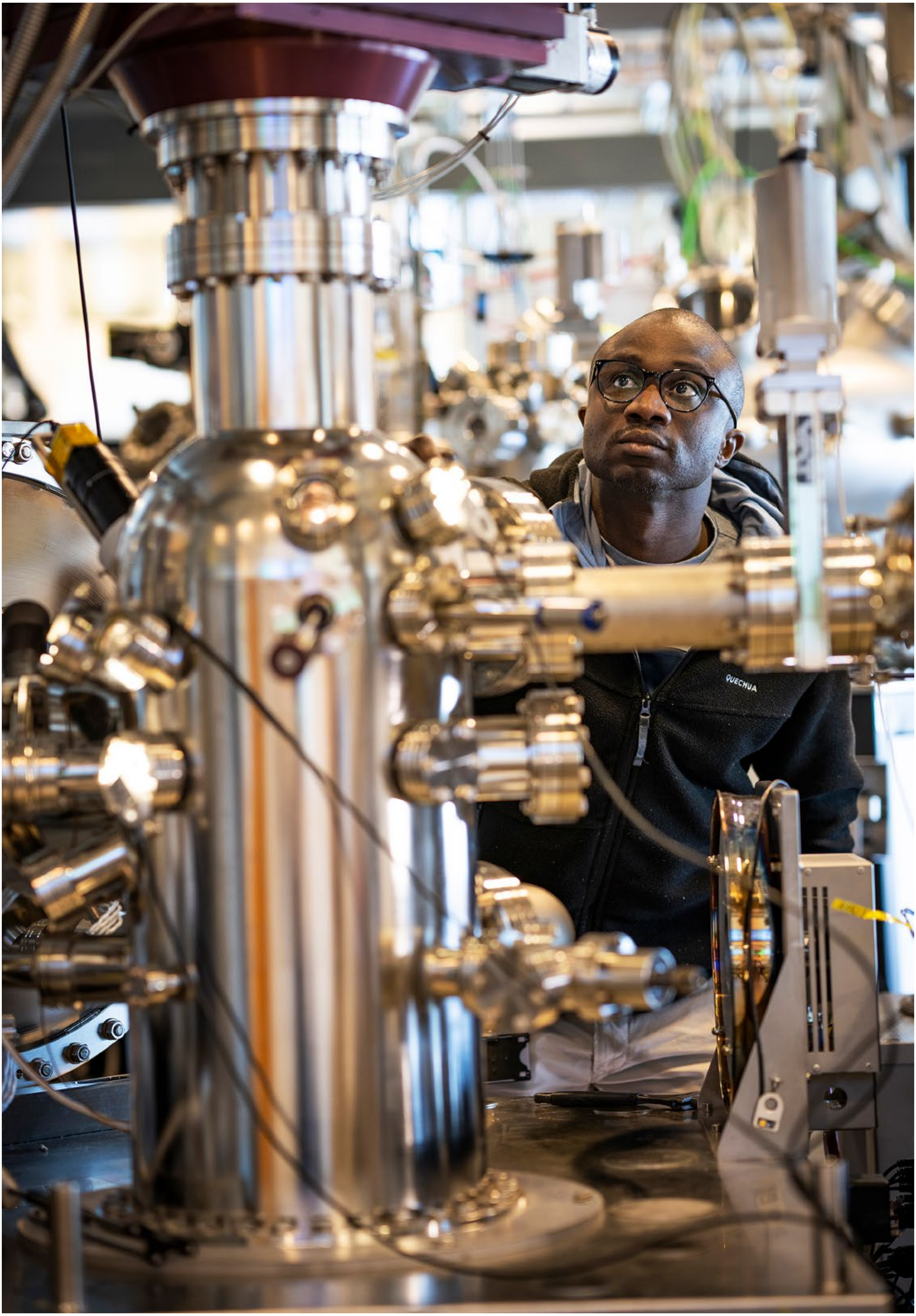


Figure 13: The "Spot" dog-robot being tested at MAX IV.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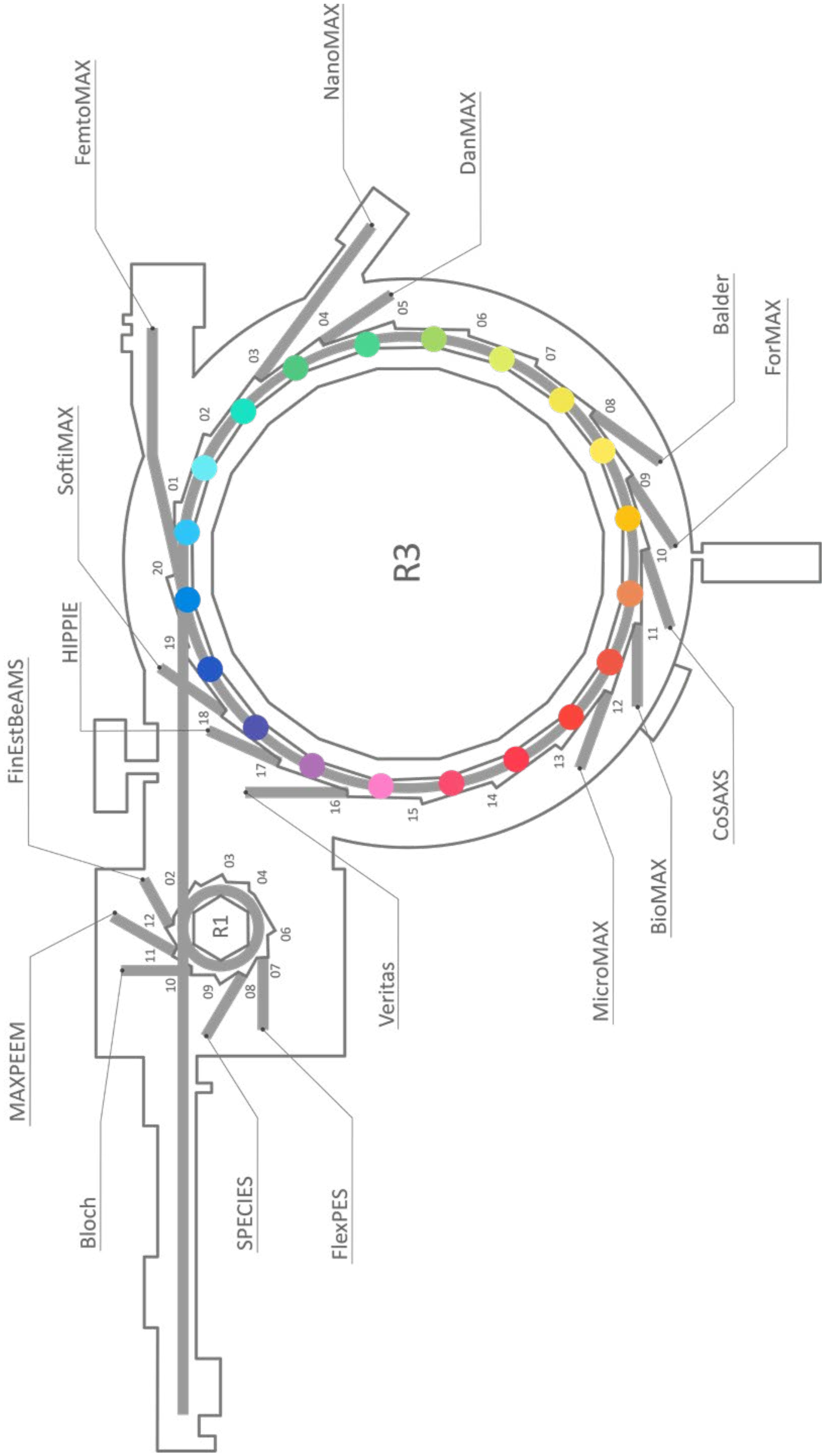
Facts and Figures



FemtoMAX
NanoMAX
DanMAX
Balder
ForMAX
CoSAXS
BioMAX
MicroMAX
Veritas
SoftiMAX
HIPPIE
FinEstBeAMS
MAXPEEM
Bloch
SPECIES
FlexPES
R3
R1

Beamline	Methods
Balder	Hard X-ray absorption and emission spectroscopy (XAS, XES) and X-ray diffraction (XRD) with emphasis on in-situ and time resolved studies
BioMAX	Macromolecular crystallography with a high degree of automation and remote user access
Bloch	Angle-resolved photoelectron spectroscopy (ARPES) including spin resolution (spin-ARPES) for studies of the electronic structure of solids and surfaces
CoSAXS	Small and wide angle X-ray scattering (SAXS, WAXS) and coherent techniques for soft matter and biomaterials
DanMAX	Powder diffraction (PXRD) and full-field tomographic imaging of hard (energy) materials
FemtoMAX	Time-resolved hard X-ray scattering (XRD) and spectroscopy (XAS) methods for studies of ultrafast processes
FinEstBeAMS	Electron and ion spectroscopies, and luminescence methods for studies of low density matter and solids
FlexPES	Soft X-ray spectroscopies for studies of low density matter and solids
ForMAX	Full-field tomography, SAXS/WAXS, scanning and imaging
HIPPIE	Ambient Pressure Photoelectron Spectroscopy (AP-XPS) on solids and liquids
MAXPEEM	Photoelectron microscopy for investigation of surfaces and interfaces
MicroMAX	Macromolecular crystallography, serial crystallography, time-resolved crystallography
NanoMAX	Imaging with spectroscopic and structural contrast techniques on the nano scale
SoftiMAX	Scanning transmission X-ray microscopy (STXM) and coherent imaging methods
SPECIES	Resonant inelastic X-ray scattering (RIXS) and Ambient Pressure Photoelectron Spectroscopy (AP-XPS)
Veritas	Resonant inelastic X-ray scattering (RIXS) with a unique resolving power and high spatial resolution

MAX IV in brief

MAX IV Laboratory is a Swedish national user facility that uses X-rays from a linear accelerator, a 1.5 GeV storage ring, and a 3 GeV storage ring, respectively. The 1.5 GeV ring focuses on softer X-rays, while the linac provides X-rays to our Short Pulse Facility. The 3 GeV ring is the first fourth-generation synchrotron storage ring and provides unprecedentedly bright, coherent, soft and hard X-ray beams because of its uniquely small emittance.

The Covid-19 pandemic continued to impact the operation of our beamlines and our projects, as described in detail in various sections of this report. Still, the laboratory continues to grow its portfolio of X-ray beamlines, with currently sixteen (16) funded beamlines. During 2021, the accelerators performed well and delivered X-rays to fourteen (14) beamlines. Thirteen (13) of these received general users via peer-reviewed access in open calls. The DanMAX beamline completed most of its commissioning plan and performed its first general user experiment in December 2021. Our Scanning Transmission X-ray Microscopy (STXM) instrument, SoftiMAX, received expert users for commissioning activities throughout 2021 and will host its first general users in early 2022. Two (2) remaining beamlines, ForMAX and MicroMAX, are in late construction. The start of their commissioning activities will be slightly delayed because of the Covid-19 pandemic and associated worldwide disruptions of supplies.

Despite this unusual year as a continuation of the impact of the Covid-19 pandemic, the laboratory held its two usual calls for proposals. The engagement of the user community remains strong. More than 45 % of our users in 2021 were from Sweden. Also, MAX IV continues to position itself regionally as serving principally scientists from northern European institutions, with more than 79 % of visitors from the Nordic area and the Baltic countries combined. We also note that the industrial use of MAX IV continued to grow substantially (more than 100 %) in 2021.

Like every year in October, MAX IV held its User Meeting, this time as a hybrid meeting. It gathered about 400 participants, half of whom attended the meeting in person. This was the opportunity to further discuss the development of our strategic process, especially after completing 16 focused strategy workshops held during the two-month time leading to the User Meeting. This led to a call for submission of Letters of Interest for major instrumentation proposals that would further guide the laboratory's strategy. More information is provided on our dedicated webpage at https://www.maxiv.lu.se/about-us/max-iv-strategy-2023-2030/.

VR also conducted a fifth project review of MAX IV in November 2021 to evaluate how the laboratory progresses toward operations. The review praised the progress made by the laboratory's beamlines and accelerators but also pointed to several areas of improvement that will be addressed during 2022.

User Programme

By the end of 2021, MAX IV consists of sixteen (16) funded beamlines, among which two (2) are under construction:

- Fourteen (14) beamlines were taking X-rays in 2021.
- DanMAX - the construction and commissioning of DanMAX progressed well during 2021, and it accepted general users in December 2021.
- SoftiMAX – The completion of the construction of the SoftiMAX Scanning Transmission X-ray Microscopy endstation supported commissioning activities throughout 2021. SoftiMAX will accept users in 2022.

- ForMAX, MicroMAX – these two beamline construction projects encountered delays because of the Covid-19 pandemic and subsequent chain supply management disruptions. They are expected to accept general users in 2023.
- The details of the extensive capabilities of our beamlines are listed in Appendix 2 but also on our website in our periodical beamline status reports: https://www.maxiv.lu.se/science/reports/

Impact of the Covid-19 pandemic on our User Programme

Throughout 2021, the Covid-19 pandemic continued to impact the regular operation of our facility in many ways by altering the execution of our User Programme (i.e., cancellation and postponing of experiments) and delaying many of our projects. Figure 6 illustrates the points described below regarding user operation status and user site access during 2021.

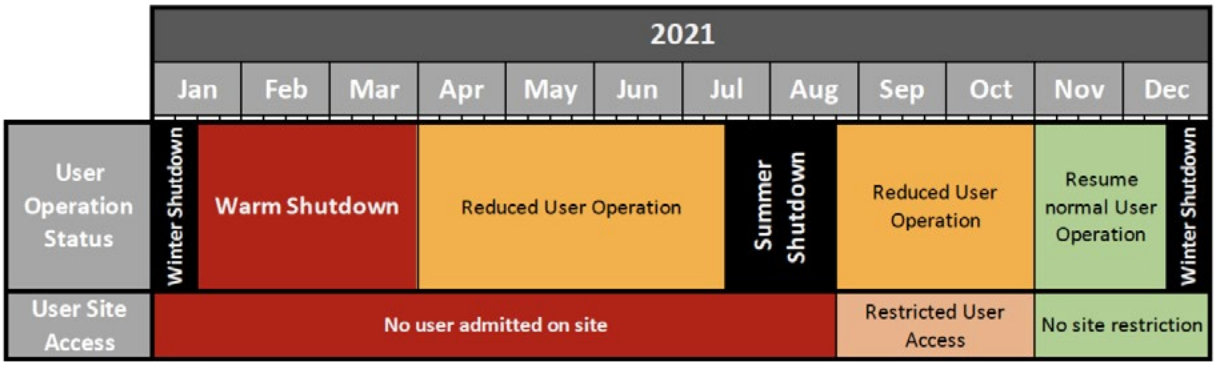


Figure 6: Description of the impact of the Covid-19 pandemic on our 2021 User Programme in terms of User Operation Status and User Site Access.

To follow the public health recommendations, MAX IV entered into a Warm Shutdown from January 18th, 2021 until March 30 th , during which the vast majority of on-site project activities and our user access were suspended. Staff access was limited to the very necessary.

This was followed by a phase of reduced operation, during which beamlines gradually resumed user operation one after another. During that time, no user access was permitted. All experiments were performed as mail-in or remotely. BioMAX, our high-throughput beamline dedicated to macromolecular crystallography, is designed to be compatible with mail-in and remote operation and resumed user operation promptly. The other beamlines evaluated each experiment on a case-by-case basis to assess the possibility or not of performing experiments in any of these two modes of operation: mail-in or remote. This possibility varied greatly from beamline to beamline and with the nature of each experiment.

During the Autumn, access to our facility was gradually restored to full access (normal operation) on November 3rd, 2021. However, international users still encountered travel restrictions, and many experiments had to be cancelled or performed remotely.

In retrospect, 2021 has been very similar to 2020. We observed the cancellation of many user experiments and performed a significant number of experiments without the physical presence of the user group.

For the statistics described in more detail below, we counted each registered user group member for a given experiment as a physical "visit." Each user registered for different experiments is thus accounted for multiple times if listed on different

experiments. Still, our User Programme Statistics for 2021 presented in this section will preclude any qualitative or quantitative comparison to previously reported data. The number of proposals submitted, accepted, and executed was heavily impacted by cancellation/re-scheduling. Also, the number of our on-site visitors is dramatically decreased.

User Programme Statistics

In Table 1 below, we provide statistics related to our User Programme for the period running from March 1st, 2021, to February 28th, 2022.

In 2021, MAX IV hosted 1203 user visits. We note that through 2021, site access was precluded most of the year because of the Covid-19 pandemic, as illustrated in Figure 6 (No site access). The distribution per beamline is indicated in Table 1. As mentioned previously, in addition to the usual definition are added those users registered on the proposal for which the experiment was conducted as mail-in or remote. The average gender distribution was 30 % women and 70 % men.

Beamline	User visits
Balder	88
BioMAX	271
Bloch	82
CoSAXS	69
DanMAX*	121
FemtoMAX*	29
FinEstBeAMS	67
FlexPES	112
HIPPIE	96
MAXPEEM	90
NanoMAX	102
SoftiMAX*	14
SPECIES	57
STM-lab	5
Veritas	0
Total	**1 203**

Table 1: User visits per beamline during the reporting period. Please note that each user registered on the proposal was counted as a visitor for those experiments that were conducted as mail-in or remote experiments.

The geographical distribution of our users' home institutions is provided in Table 2 and Figure 7. The majority of our users were from Sweden with 49 %, followed by Denmark with 20 % and Finland with 4 %. This further highlights the solid regional position of MAX IV as a leading X-ray user facility serving a user community centrally located in northern Europe but most notably in the Nordic and Scandinavian regions.

Region	User visits
Sweden	49 %
Scandinavia (Sweden, Denmark, Norway)	71 %
Nordic (Scandinavia, Finland, Iceland)	75 %
Northern Europe (Nordic, Baltic countries)	79 %
Europe	96 %

Table 2: Regional geographical distribution of user visits.

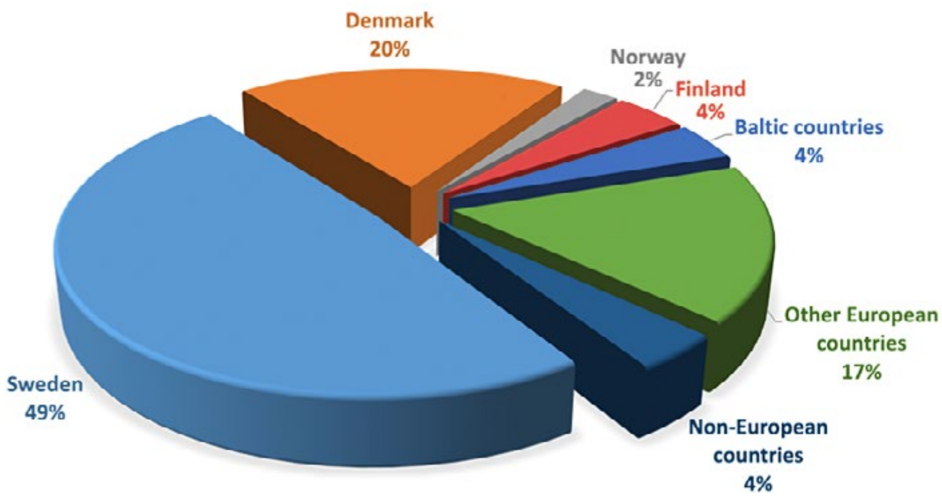


Figure 7: Geographical distribution of the home institution for the recorded user visits for the reporting period.

Industry Engagement

An industry strategy was developed by the Industrial Relations Office (IRO) during the second half of 2020 and approved in March 2021 by the MAX IV board. This strategy focuses on a sector-based initiative approach with four central goals: (i) broaden the industrial user base, (ii) increase the industrial use of MAX IV, (iii) develop MAX IV to support industrial needs, (iv) use a collaborative approach to industry engagement.

This strategy guides industry activities and actions over the coming years and is part of the

facility's strategic plan. We have identified ten (10) industry sectors for which the X-ray-based analytical techniques available at MAX IV have a solid potential for impactful industrial research and development. We are actively working on a subset of those sectors with various initiatives to strengthen possibilities to take advantage of the uniqueness of our research infrastructures.

In 2021, the number of industrial users is more than doubled compared to 2020. The amount of proprietary beamtime purchased from MAX IV also nearly doubled. In total, 556 hours of proprietary beamtime were purchased by twenty-seven (27) companies and institutes on seventy (70) occasions during 2021. Table 4 highlights the progression of industrial use of MAX IV since 2018 and provides the breakdown per technique in hours. For each X-ray technique, the respective MAX IV beamlines involved in these beamtimes are listed.

A third of the proprietary beamtime in 2021 was connected to Vinnova pilot projects. A more significant number of companies used MAX IV through the Vinnova pilot project funding, and we also observed an increased number of mediators from academia and institutes.

Industry users	2018	2019	2020	2021
Total industry users	4	13	11	27
New industry users	4	10	7	18
Mediators (private, institute, acacemic*	1	4	4	10*
Total proprietary beamtime [hours]	43	216	313,5	556
MX (BioMAX)	43	132	218	300
Spectroscopy (HIPPIE, Balder)		60	34,5	140
Imaging (NanoMAX, MAXPEEM)		24	37	96
Scattering (CoSAXS)			24	20

*Table 4: Number of industry users, new industry users, and proprietary beamtime utilization in hours of MAX IV in 2021. *Two (2) private mediator companies, three (3) institutes, and five (5) academic mediators*

MAX IV was nearly shut down during the first half of 2021 because of the Covid-19 pandemic. The unusual character of the pandemic renders the analysis of this year's statistics challenging to support any substantial analysis regarding future trends. However, we note that the general user access mode (i.e., in collaboration with academic partners through open research projects) remains an important channel for the industrial use of MAX IV.

In January 2021, the IRO team expanded with a full-time member in collaboration with Alfa Laval. This two-year assignment aims to examine how to develop and increase the engagement and commitment to using MAX IV from the R&D activities of the Nordic metal industry. During the first year, the work was focused on understanding the needs of the metal industry and identifying the crucial elements necessary to generate a long-term engagement from both a technical and a business perspective. Also, this was complemented by various forms of workshops and discussions organized with several Swedish companies. Several gaps and areas of improvement have been identified and are used to inform the basis for updating our strategy for future actions.

A new VR-funded project, InfraLife, started at the beginning of 2021. It aims to establish a joint hub between three large-scale research infrastructures: MAX IV, ESS, and SciLifeLab, and to create better access opportunities to the life science industry and health care sector in Sweden.

The project adopts a challenge-driven and knowledge exchange approach between the infrastructures. During the spring of 2021, a project addressing anti-microbial resistance resulted in a workshop gathering major stakeholders and during which challenges and opportunities were discussed. The project also focused on mapping ongoing activities, generating outreach materials, and laying the foundation for the activities to be developed in the future.

The Northern Lights on Food (NLF) initiative continued supporting various activities that gather organizations from industry, academia, research institutes, and the industry sector. In June 2021, more than one hundred (100) participants attended the second NLF conference. In November 2021, a second Master Class in food science at synchrotrons focused on imaging techniques and attracted academic and industrial researchers. The Lund Institute of advanced neutron and X-ray science also launched a Northern Light on Food theme, further strengthening the initiative: https://www.linxs.se/northern-lights-on-food

The MAXESS Industry Arena project continued growing with new partners, and new features are available on the website (https://maxess.se/). Vinnova pilot projects are presented as "easy to read" industry cases on the website as examples

of how industry can benefit from large-scale research infrastructures. SmiLe Life Science Incubator joined the project with funding from the EU (regional funds) and Region Skåne to develop a process to connect stepping-stone environments such as SmiLe into the eco-system of service providers around MAX IV and ESS. The project was awarded funding for two years starting from mid-2021.

The collaboration with RISE and Swerim continued through a VR-funded initiative. Partnerships with their staff, MAX IV beamlines, and the MAX IV user community took many forms, including beamline development and commissioning, engagement in the MAX IV strategy process, industry user beamtime, outreach activities, and other joint project activities.

Collaborations and partnerships

By the end of 2021, MAX IV was involved in fifty-three (53) externally funded projects from fourteen (14) funding agencies for a total contract amount of 192 972 656 SEK. Details are provided in Figure 23.

MAX IV is the project leader in twenty-one (21) of these external projects and received funds for twenty-three (23) additional projects as a collaborator. For nine (9) external projects, there are no funds for MAX IV, and the facility´s participation is in-kind.

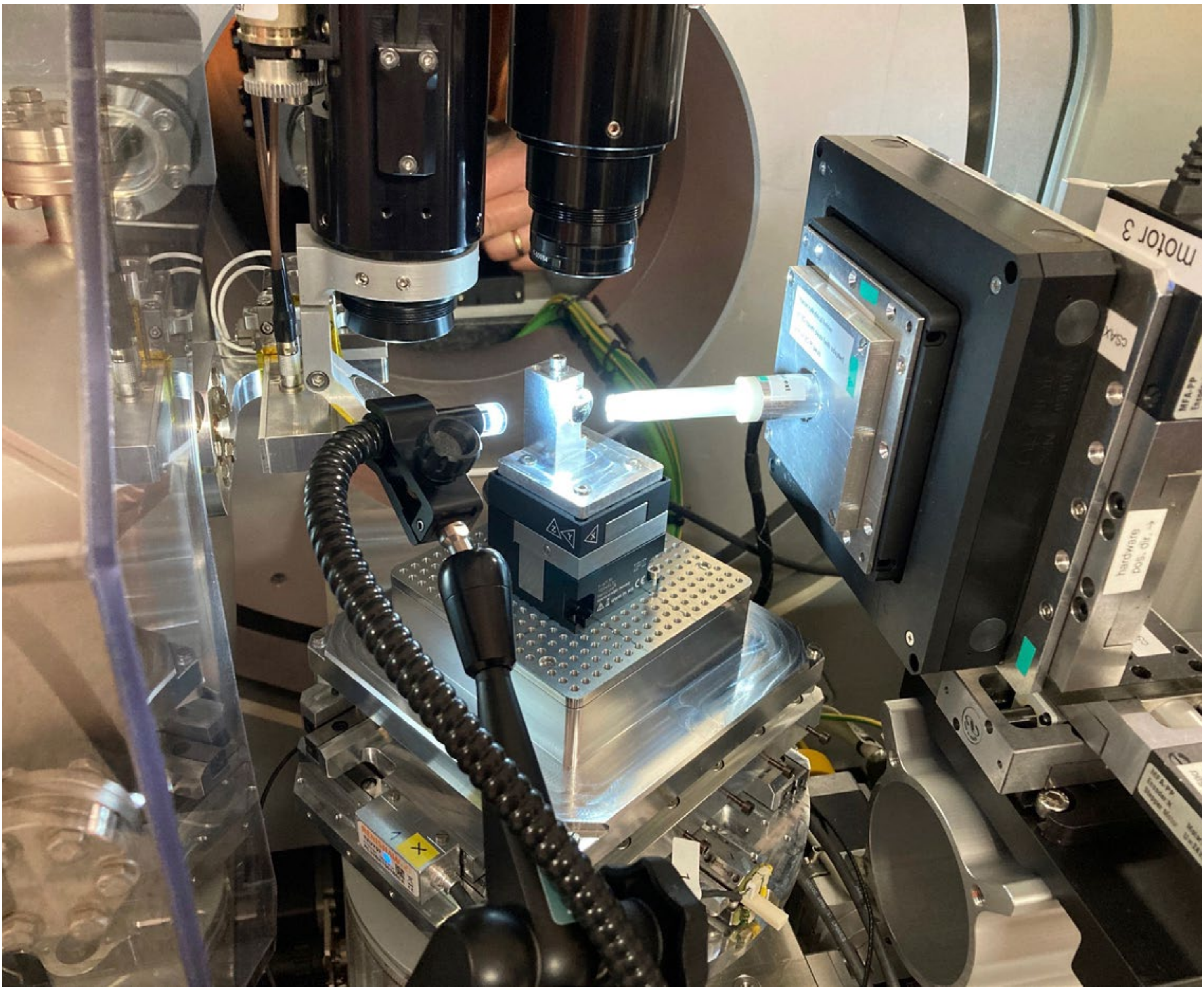
We also note that MAX IV reached its highest involvement in projects funded by the European Commission, with seven (7) active projects in 2021.

Twenty-seven (27) new external projects started in 2021, some of which received a funding decision in 2020. MAX IV is the project leader for twelve (12) of these projects. As a collaborator, MAX IV also received funds for ten (10) additional and is involved in five (5) more projects for which no funds are transferred to MAX IV.

We specifically highlight three (3) projects that were approved in the framework of the VR Grant for investment in existing research infrastructure:

▶ Collective dynamics with coherent X-rays

This funded project was directed towards developing the use of X-ray coherence by procuring a state-of-the-art detector for fast time-resolved X-ray photon correlation spectroscopy (XPCS) in collaboration with the user community.



▶ TRISS – Trapped Ion Spectrometer Setup
This funded project aimed at developing a set of internationally unique and competitive instrumentation that facilitates trapped ion x-ray spectroscopy. This is relevant for many scientific areas: molecular physics, biomolecular research, clusters/super-atoms, energy materials, atmospheric chemistry, astrophysics, astrochemistry, astrobiology, and surface physics.

▶ Upgrade of the AC-SPELEEM microscope with a new energy analyzer and detector of electrons
This funded project will improve the performance of the existing MAXPEEM beamline and attract new users inside and outside Sweden by implementing a new energy analyzer with an increased energy resolution and a state-of-the-art electron detector.

MAX IV continues to network with various external collaborations actively. MAX IV is part of large networks on an international level, such as the League of European Accelerator-based Photon Sources (LEAPS), lightsources.org, and the Analytical Research Infrastructures in Europe (ARIE). Such collaborative environments are platforms promoting the exchange of information and knowledge, which is often the trigger of project applications that creates consortia applying for funding at the EU level.

On a national level, MAX IV interacts with various networks such as Treesearch, Northern Lights on Food, Metalbeams, etc. This contributes to strong collaboration with Swedish academia and industry that allows us to further guide our facility's development while ensuring Swedish research remains at the forefront of science.

Finance

In 2021, the MAX IV operating budget was funded by Vetenskapsrådet (aka the Swedish Research Council, VR), Vinnova, Formas, 14 Swedish universities (Chalmers Tekniska Högskola, Göterborgs universitet, Karlstads universitet, Karolinska Institutet, Kungliga Tekniska Högskolan, Linköpings universitet, Linnéuniversitetet, Luleå tekniska universitet, Lunds universitet, Malmö universitet, Sveriges lantbruksuniversitet, Stockholms universitet, Umeå universitet, and Uppsala universitet) and an additional contribution from Lund University. We also note that Finland and Estonia contributed to our operating budget, thus reflecting their continued strong commitment to their collaboration with our facility.

In September 2020, RFI (aka the Council for Research Infrastructures within the Swedish Research Council) requested material from MAX IV for informing its upcoming decision regarding the funding period 2023-2026. Furthermore, RFI plans to take an indicative funding decision for 2027- 2030. A budget request was incorporated in the first draft for the MAX IV strategic plan for the same period and was submitted in March 2021.

Comments on the outcome of the 2021 MAX IV Operating Budget

Details regarding funding, costs and results are provided in the MAX IV Annual Report. MAX IV delivered a result of -20.6 MSEK and hence a corresponding decrease in agency capital. The outgoing agency capital in 2020 was 35.1 MSEK.

The budgeted change in undepreciated funds (+ 31 MSEK) was increased by 27.1 MSEK to 58.1 MSEK, mainly due to lower overall spending in all groups, as a direct result of the Covid-19 pandemic.

The adjustment of the planning for beamline, accelerator, and infrastructure projects contributed to delays in budgeted investments, procurements, and delayed deliveries which also included a lower depreciation.

Recruitments progressed according to the staffing plan and were negligibly impacted. The MAX IV post-doctoral program, previously interrupted at the end of 2019, resumed in 2021. Staff increase was strategically directed towards increasing our level of user support, ultimately working toward providing 24/7 user support with the addition of floor coordinators, a practice that has been successful at other facilities of similar nature. All budgeted positions in 2021 have been filled except for a few exceptions. We note that several filled positions will have an employment starting date in 2022.

Organisation and staff

At the end of 2021, MAX IV consisted of 279.5 full-time employees. MAX IV continues to steadily grow as an organization while constructing, commissioning, and operating an increasing number of beamlines. Most of our open positions are advertised internationally to seek the strongest possible candidates, thus resulting in about half of our employees being from countries other than Sweden.

The search for a permanent Physical Sciences Director initiated in autumn 2020 concluded. Following the recommendation from the MAX IV Director to the MAX IV Board, the recruitment of a Physical Sciences Director was completed in 2021. Dr. Aymeric Robert started full-time employment on October 4, 2021.

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