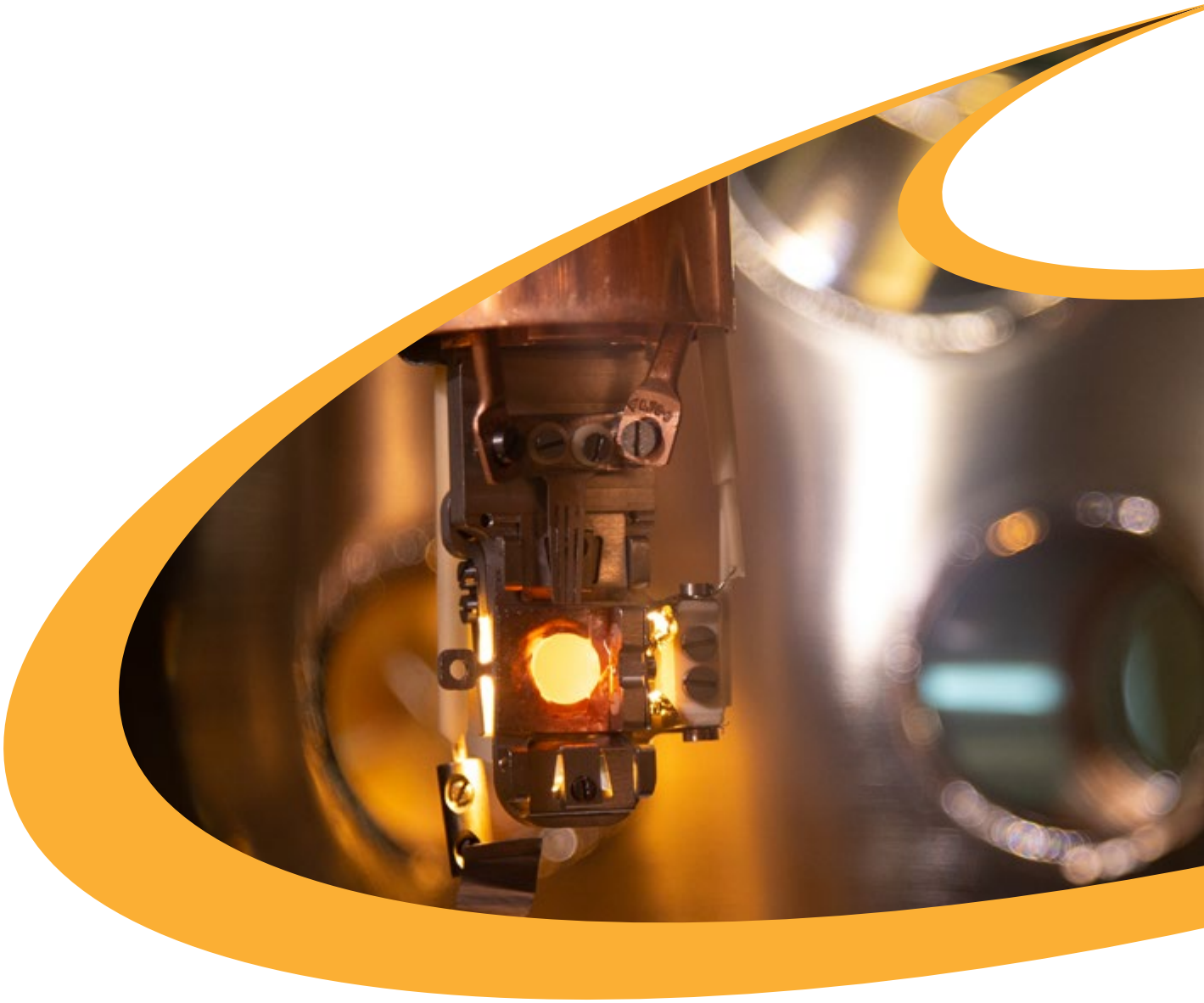
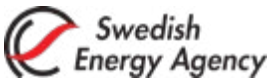
HIGHLIGHTS 2020



MAX IV

Partners



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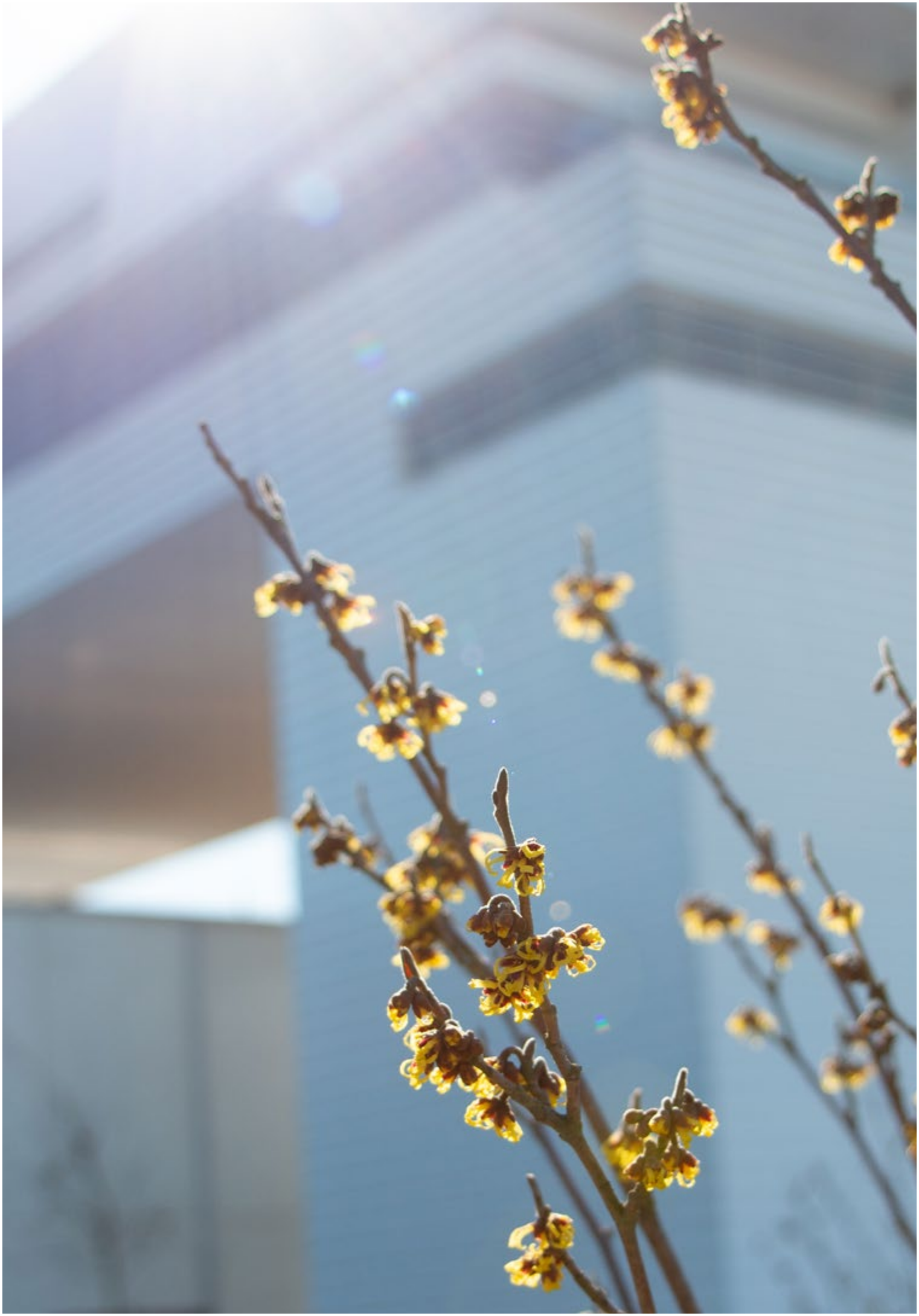


Foreword

MAX IV rose to new heights in 2020 – an auspicious year for the Laboratory. Two new beamlines saw "first light", SoftiMAX with a scientific program focusing on soft X-ray microscopy and coherence experiments, and DanMAX on hard X-ray powder diffraction and 3D imaging studies. Both beamlines hosted their first expert users as part of commissioning activities. MAX IV also moved well into user operations on its other beamlines in 2020. By the end of the year, eleven beamlines welcomed general users, bringing the total number of beamlines in user operation and commissioning to fourteen of the sixteen funded.

2020 also brought the COVID-19 pandemic. The growing concerns of infection and ensuing travel restrictions, both within Sweden and without, significantly impacted the MAX IV user science programs, mainly because many users were unable to travel to MAX IV for their scheduled beamtime. Nevertheless, MAX IV supported many experiments by users who could travel as well as a substantial number of experiments through mail-in services and remote operations. Development of these capabilities was never envisioned for most beamlines (as elsewhere worldwide). Their rapid implementation and effectiveness in carrying forward the beamline science programs is a testament to the ingenuity and hard work of the MAX IV staff. While the statistics for 2020 cannot be compared to pre-pandemic years, MAX IV hosted 1036 user visits and 560 individual users in mail-in or remote mode by the end of the year. About 56% of the user proposals allocated beamtime in 2020 were authored by researchers based at Swedish institutions, reflecting a continuation of the healthy balance of domestic and international user communities.

Innovations in the operation of MAX IV's accelerators in 2020 complemented the innovations on the beamlines. These included achieving and surpassing operational goals for beam delivery, beginning regular linac operation at 10 Hz repetition rate, enabling inauguration of the FemtoMAX user program at 10 Hz, near-transparent injection of the rings, and in the spring of 2020, measurement of sub-micrometer beam perturbations. In addition, the thermal stability of the beamlines was improved by top-up injection every 10 min by comparison to the previous interval of 30 min. These innovations enabled new user and staff science, as can be seen in a dramatic growth in the scientific output of MAX IV.

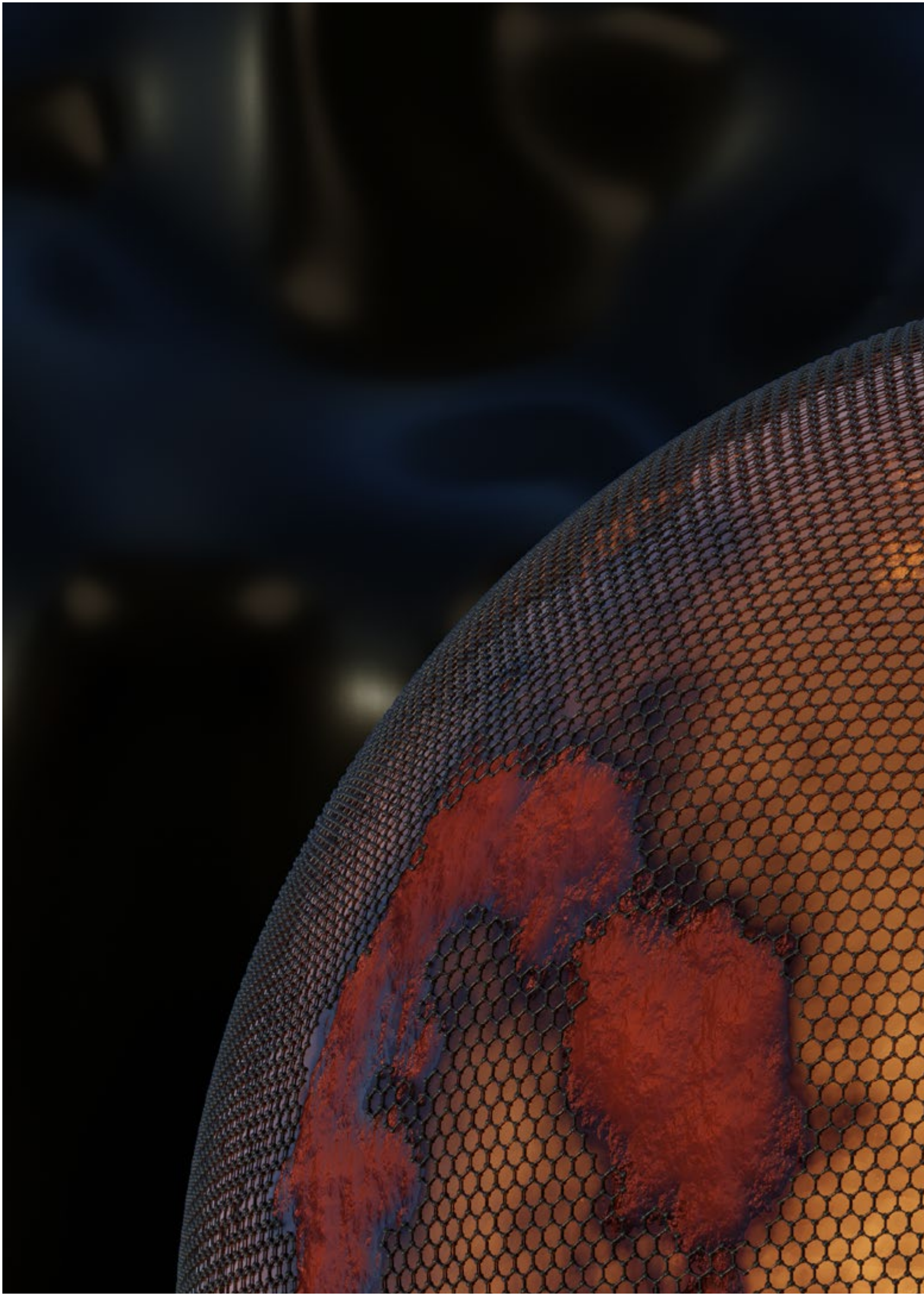
MAX IV users and staff published 112 scientific articles in 2020. A growing number can be found in high-impact journals, reflecting the growing impact and recognition of the quality of the results arising from the Laboratory. Exciting examples that you can read about in this volume include advanced materials for electronics, energy storage and corrosion protection, durable human-made wood, efficient catalysts for the production of essential chemicals, cloud formation affecting climate modelling, a way to compensate for nanoparticles not sitting still in the X-ray beam, gut microbiome, bone formation, as well as new insights for antibiotic resistance and cancer.

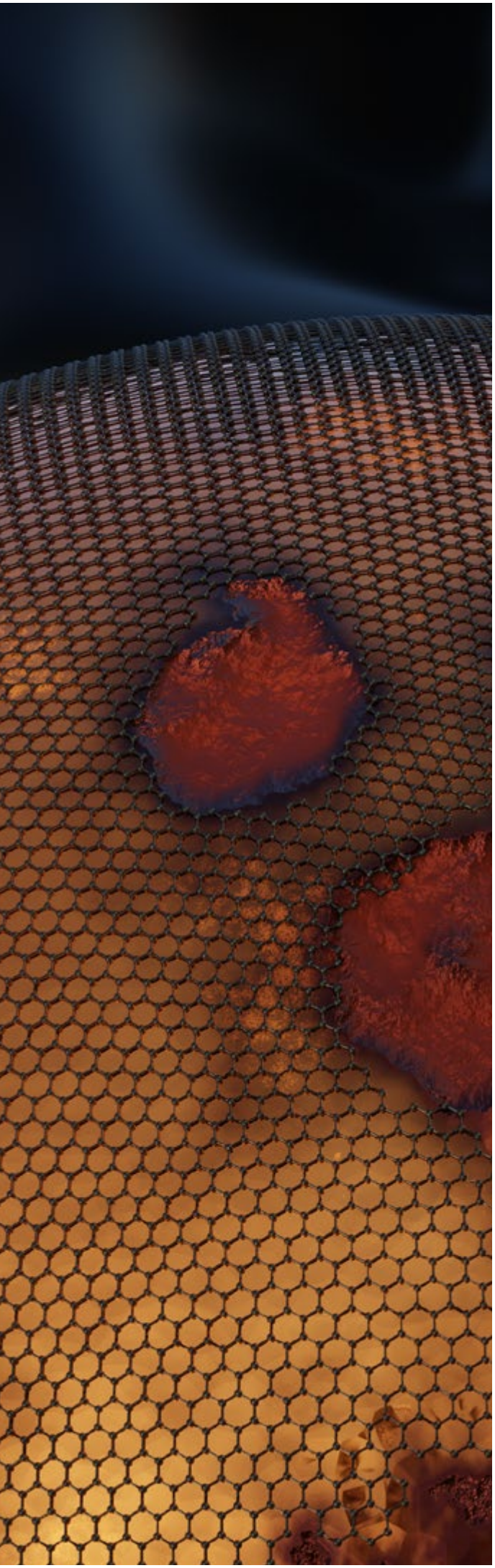
I would like to thank the MAX IV staff and users for making these outstanding results possible. Their huge effort enabled the Laboratory to adapt during the pandemic and continue advancing through 2020. This was no small challenge.

I also wish to give special thanks to everyone who contributed to this year's edition of MAX IV Highlights. I hope you find it inspiring to read about the excellent science resulting from activities at MAX IV. And, I hope to see you soon at the beamlines, workshops, and future user meetings!

Ian McNulty
MAX IV Director

Science Highlights





ADVANCED MATERIALS

2D-materials protecting copper against corrosion

A team led by researchers from the HIPPIE beamline at MAX IV have found that the onset temperature for copper oxidation can be increased by more than 120 °C if it is covered with graphene or hexagonal boron nitride. While a bare copper surface degrades quickly already near room temperature in an oxidizing atmosphere.

They also found that the molecular-scale mechanism of the protection is different for the two coverings due to the intrinsic properties of graphene, which is a conductor, and hexagonal boron nitride, an insulator. The team used the ambient pressure cell at HIPPIE for X-ray photoelectron spectroscopy at environmental pressure (APXPS).

The high X-ray intensity allowed following the chemical reactions in real-time with a very high energy resolution. Metal corrosion is of extreme importance as the estimated global cost of corrosion of the order of 3% of the global GDP.

Publication

M. Scardamaglia, V. Boix, G. D'Acunto, C. Struzzi, N. Reckinger, X. Chen, A. Shivayogimath, T. Booth, J. Knudsen, Comparative study of copper oxidation protection with graphene and hexagonal boron nitride, Carbon 171, 610 (2020), DOI: 10.1016/j.carbon.2020.09.021

ADVANCED MATERIALS

Aligning nanocellulose fibres for durable humanmade wood

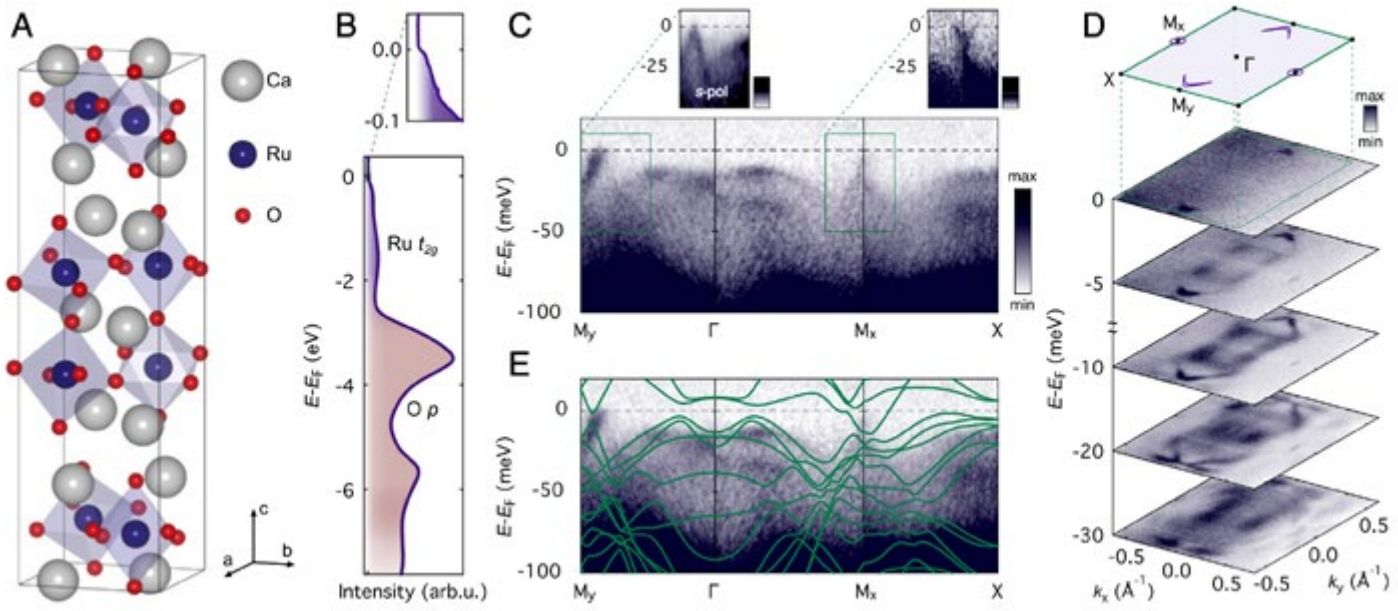
Humanmade wood composites are favoured for their customizable nature and predictability properties. A group of researchers from the University of Oulu, Luleå University of Technology, Research Institutes of Sweden (RISE), and the University of Toronto created bio-mimetic wood using an ice-templating method on nanocellulose fibres to create a similar structure to the wood cells. They recreated the hierarchical wood structure and aligned the nanocellulose fibres within the cell wall.

After drying, the result was a porous network of aligned nanocellulose fibres to be filled with epoxy resin by vacuum infusion to form a composite material. It is essential that the cellulose nanofibers are aligned in the loading direction to increase the material's mechanical properties. Furthermore, the adhesion between the cellulose nanofibers and epoxy resin is also crucial for optimal material properties.

To check the cellulose fibre alignment, the researchers used the WAXS method at the NanoMAX beamline. This study shows that the ice-templating method is a promising way for sustainable composites and new humanmade wood materials.

Publication

T. Nissilä, J. Wei, S. Geng, A. Teleman, and K. Oksman, Ice-Templated Cellulose Nanofiber Filaments as a Reinforcement Material in Epoxy Composites, Nanomaterials 11, 490 (2021), DOI: 10.3390/nano11020490



ADVANCED MATERIALS

Control of magnetic ordering in solid materials

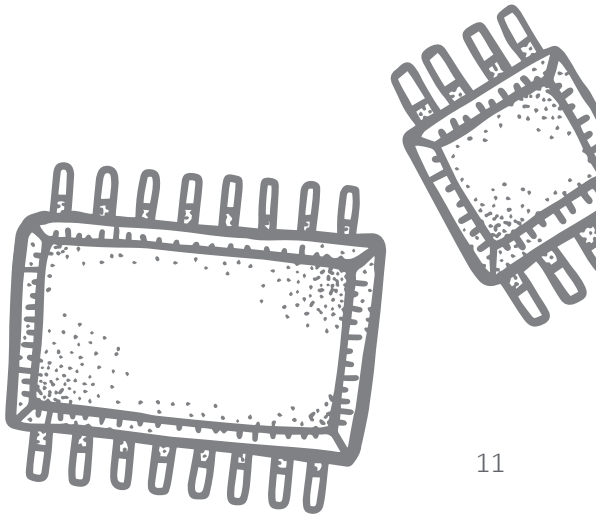
The metallic electronic states of transition metal oxide (TMO), Ca3Ru2O7 are the driver in spin-reorientation phase transition, according to research led by the University of St. Andrews in the U.K. The phenomenon, termed magneto-electronic anisotropy, provides a new method for controlling magnetic order in solid materials.

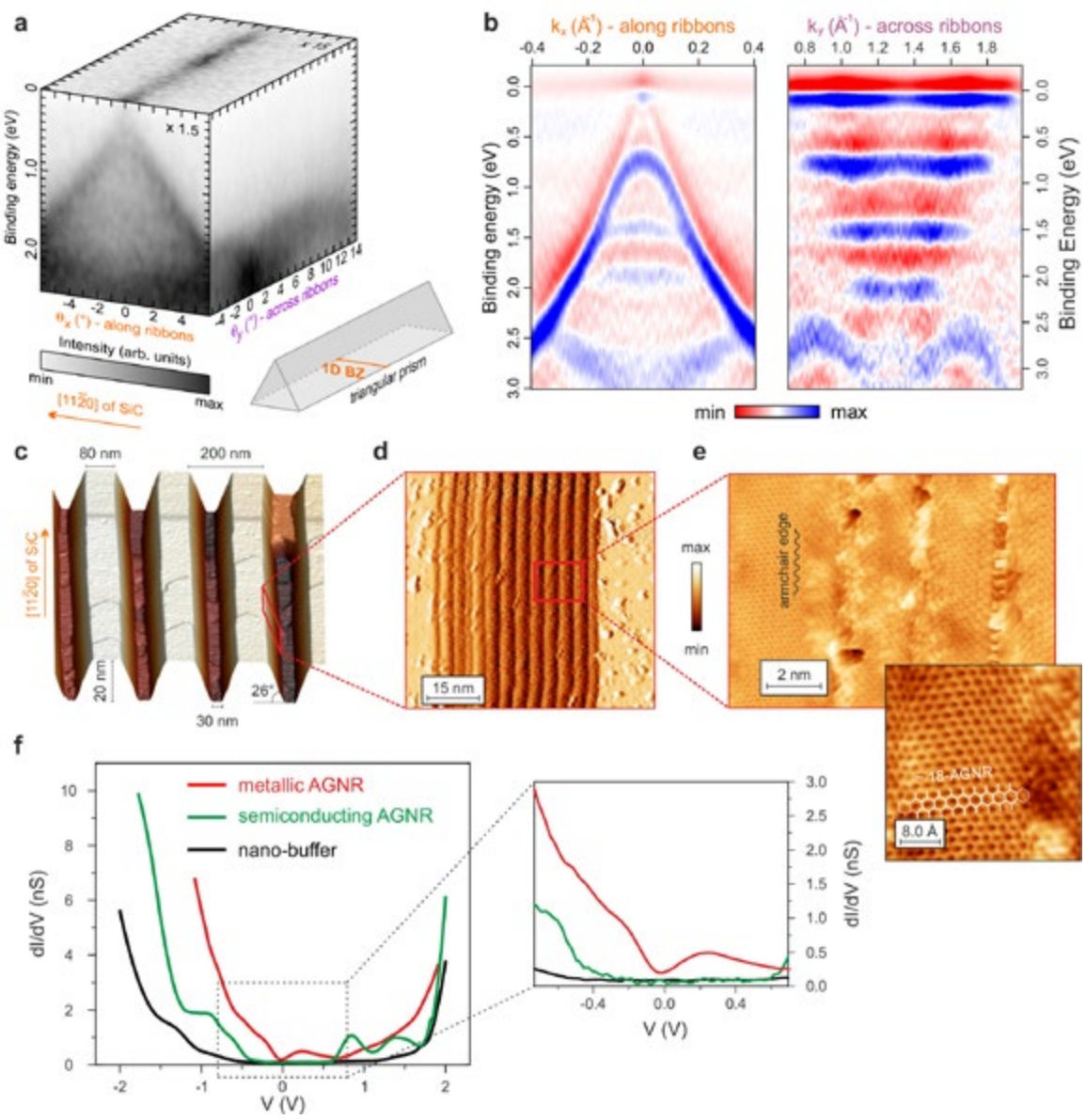
This is possible because of an interplay between structural properties and spin-orbit interactions—a relativistic coupling between the electron spin and its motion. The group investigated the temperature-dependent electronic structure of the TMO, with a focus on phase transitions happening at two different temperatures.

Angle-resolved photoemission spectroscopy (ARPES) measurements were taken at Bloch beamline at MAX IV. Fundamental understanding of magnetic ordering and how to develop stable and controllable magnetic states in materials are of enormous importance for a variety of memory and spintronic technologies.

Publication

I. Marković, M. D. Watson, O. J. Clark, F. Mazzola, E. Abarca Morales, C. A. Hooley, H. Rosner, C. M. Polley, T. Balasubramanian, S. Mukherjee, N. Kikugawa, D. A. Sokolov, A. P. Mackenzie, and P. D. C. King, Electronically driven spin-reorientation transition of the correlated polar metal Ca_3Ru2O_7. PNAS 117, 15524, DOI: 10.1073/pnas.2003671117





ADVANCED MATERIALS

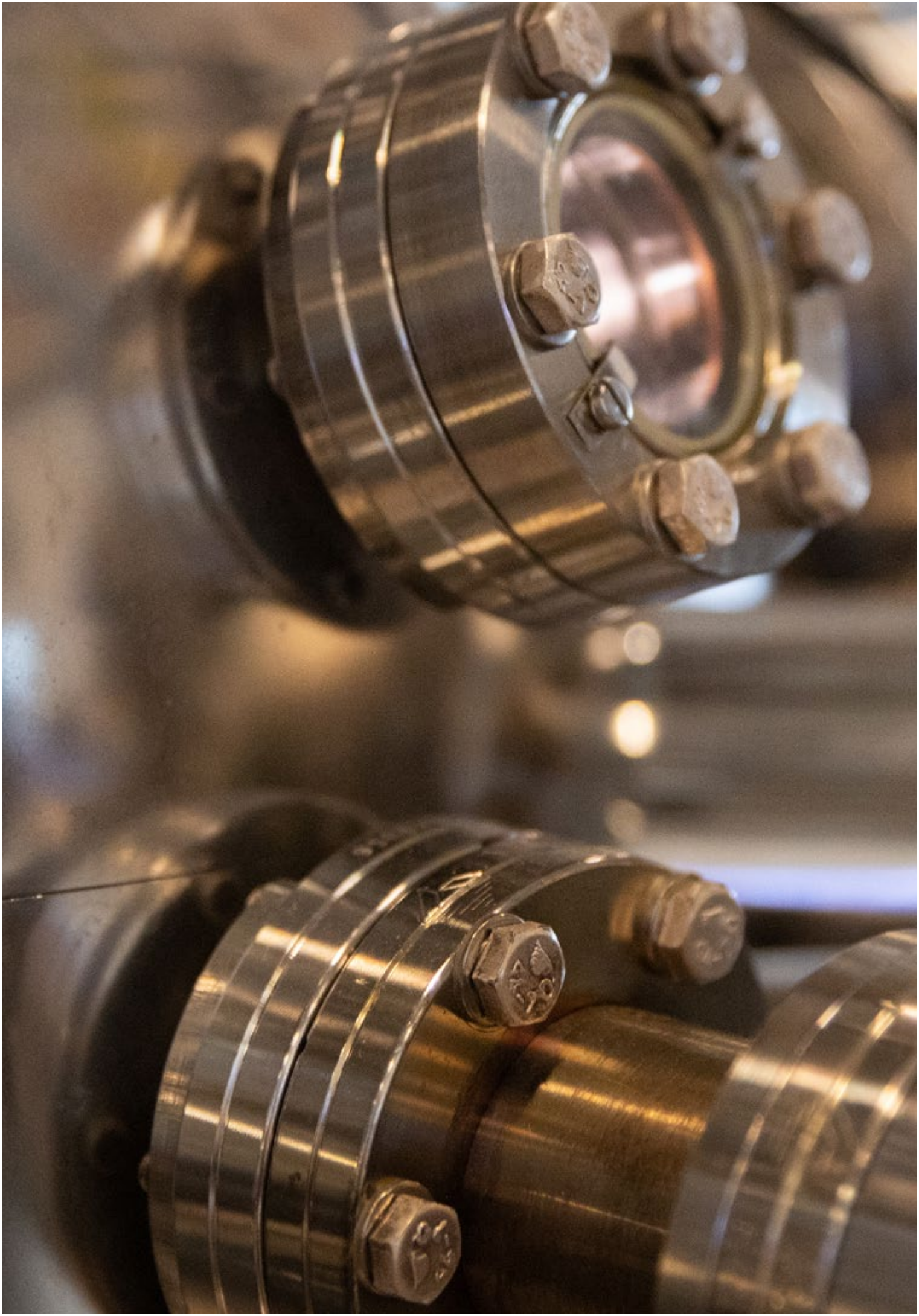
Scalable growth of graphene ribbons for nanoelectronics

Scientists looked at the electronic properties of armchair graphene nanoribbons (AGNRs) grown on the sidewalls of silicon carbide and determined a scalable approach for growing AGNRS successfully on a semiconducting substrate—a key developmental step towards improved graphene-based complementary metal-oxide-semiconductor (CMOS) technologies. The results are part of a project collaboration between Max Planck Institute for Solid State Research, the Institute of Physics at Chemnitz University of Technology, IFM at Linköping University and the School of Physics at Trinity College Dublin.

High-resolution ARPES measurements at MAX IV's Bloch beamline enabled mapping, for the first time, the electronic band structure of the ribbons. Graphene nanoribbons are intriguing for their potential use in next-generation integrated nanoelectronics. With global data traffic increasing exponentially comes the need for more powerful computational resources, which require new materials with beneficial electronic properties and miniaturization potential, for example, new transistor design concepts.

Publication

H. Karakachian, T. T. N. Nguyen, J. Aprojanz, A. A. Zakharov, R. Yakimova, P. Rosenzweig, C. M. Polley, T. Balasubramanian, C. Tegenkamp, S. R. Power, and U. Starke, One-dimensional confinement and width-dependent bandgap formation in epitaxial graphene nanoribbons. Nat Commun **11**, 6380 (2020). DOI: 10.1038/s41467-020-19051-x



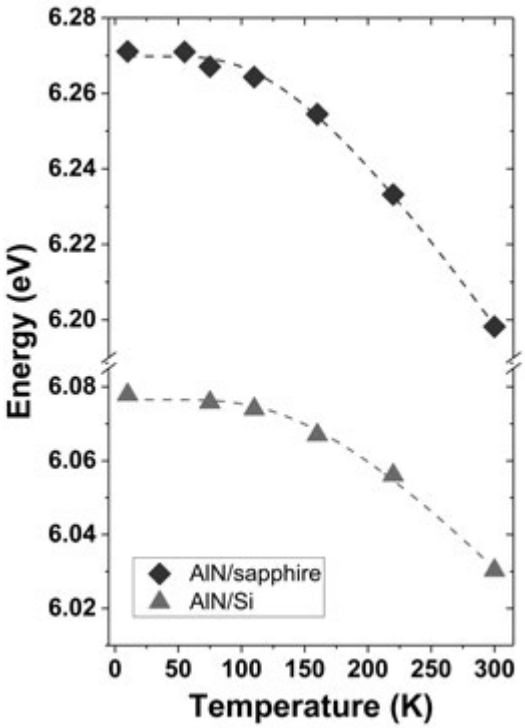
ADVANCED MATERIALS

Grasping the AlN excitonic bandgap

Ultraviolet (UV) LEDs have prime applications for sterilization, water treatment, communications, high-density optical data storage, and many others. Its durability, efficiency, and price point are the fundamental properties that make it a potent replacement for the progressively eliminated and toxic mercury lamps and inefficient gas lasers.

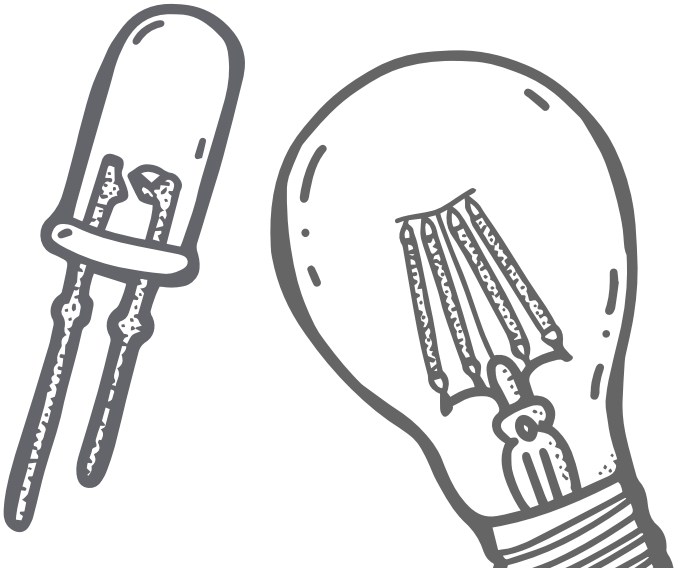
However, claiming complete control over aluminium nitride's (AlN) basic properties (the prime material for obtaining wide-bandgap barriers in nitride-based quantum structures for deep UV-emitters) is still challenging. This has motivated researchers from the Polish Academy of Sciences to conduct defect-related photoluminescence (PL) and photoluminescence excitation (PLE) spectroscopy of AlN using the FinEstBeAMS beamline.

Based on the experiments, they found that the AlN bandgap is closely dependent on the substrate. When compared to its DFT calculations, it was apparent that the tetragonal strain related to the lattice mismatch between the substrate and the AlN layer on the spectral positions of the intrinsic excitons influenced the AlN bandgap on the substrate.



Publication

A. Kaminska, K. Koronski, P. Strak, A. Wierzbicka, M. Sobanska, K. Klosek, D. V. Nechaev, V. Pankratov, K. Chernenko, S. Krukowski, and Z. R. Zytkiewicz, Defect-related photoluminescence and photoluminescence excitation as a method to study the excitonic bandgap of AlN epitaxial layers: Experimental and ab initio analysis. Appl. Phys. Lett. **117**, 232101 (2020), DOI: 10.1063/5.0027743



ADVANCED MATERIALS

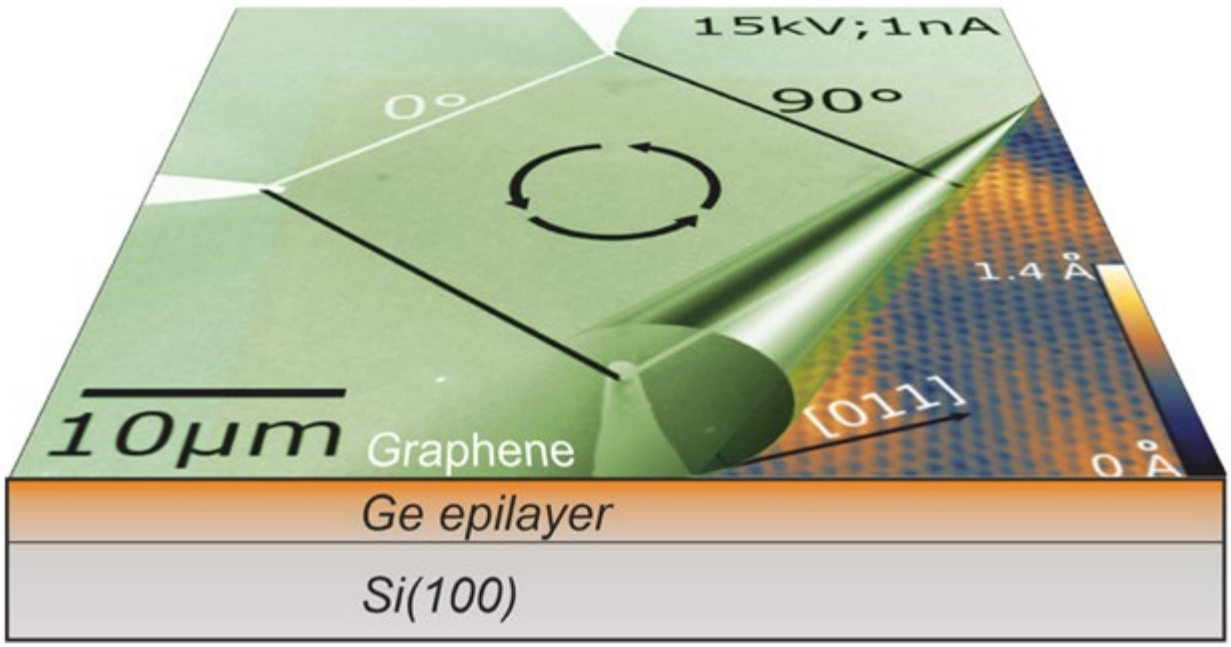
Electronic performance in focus for graphene applications

The electronic properties of 2D material graphene are a next-level benefit which scientists are beginning to unlock. A research group led by the Technical University of Chemnitz in Germany looked at structural, electronical, and transport properties of epitaxial graphene on a complementary metal-oxide semiconductor (CMOS)-compatible, germanium-silicon substrate. With in situ annealing, recondensation of the germanium surface occurred, which contributed to significant charge carrier mobility across graphene structures, even despite structural imperfections. This is primarily due to charge neutrality within the graphene films.

The electronic performance supersedes classically used silicon-carbide compounds in microelectronic and optoelectronic applications. The band structure was measured with momentum-resolved photoemission electron microscopy (k-PEEM) at the imaging beamline MAXPEEM at MAX IV. The work brings development of scalable, electronic CMOS-based applications with graphene, such as faster environmentally friendly computer chips, closer to fruition.

Publication

J. Aprojanz, Ph. Rosenzweig, T. T. Nhung Nguyen, H. Karakachian, K. Küster, U. Starke, M. Lukosius, G. Lippert, A. Sinterhauf, M. Wenderoth, A. A. Zakharov, and C. Tegenkamp, High-Mobility Epitaxial Graphene on Ge/Si(100) Substrates. ACS Appl. Mater. Interfaces **12**, 43072 (2020), DOI: 10.1021/acsami.0c10725

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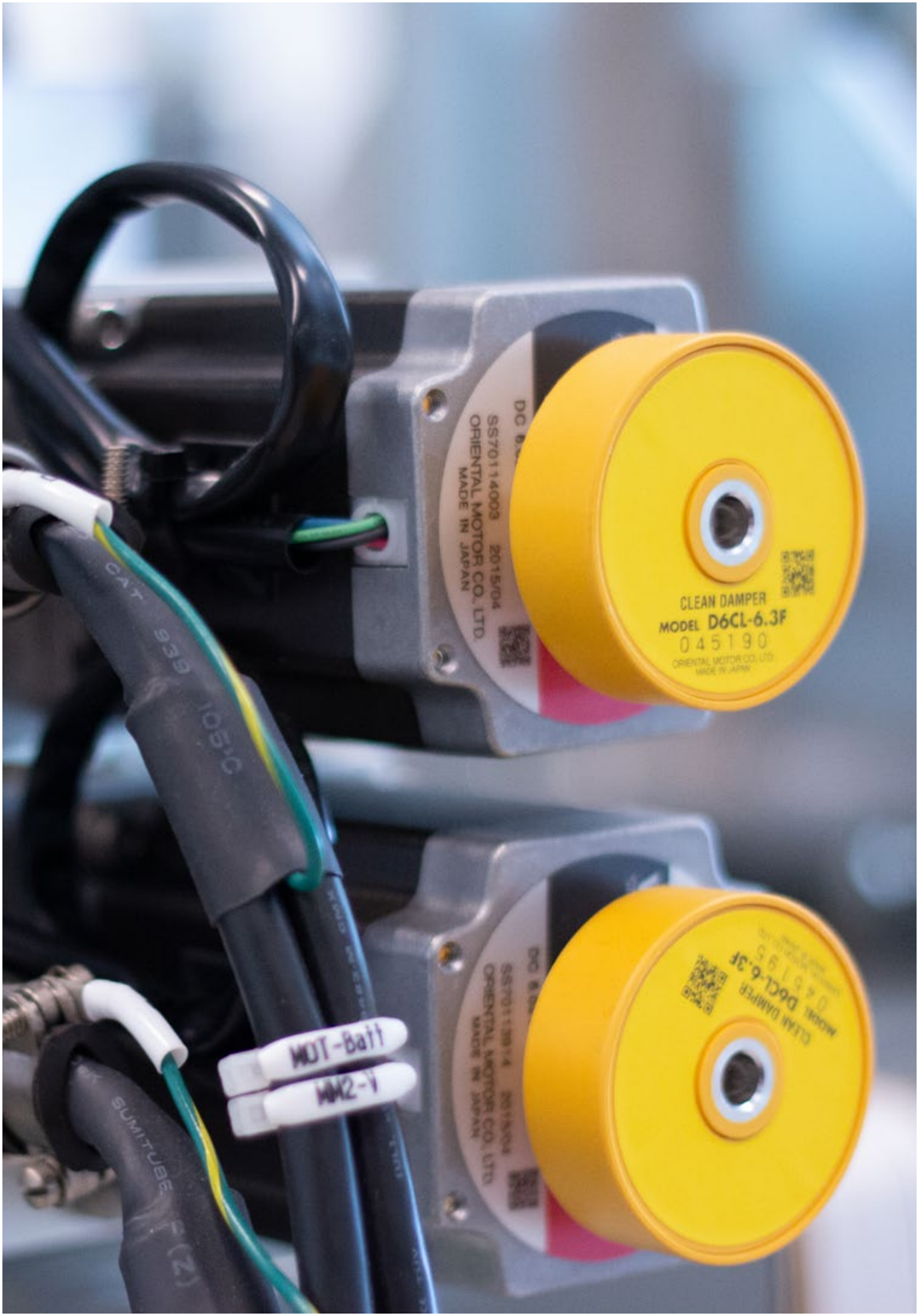
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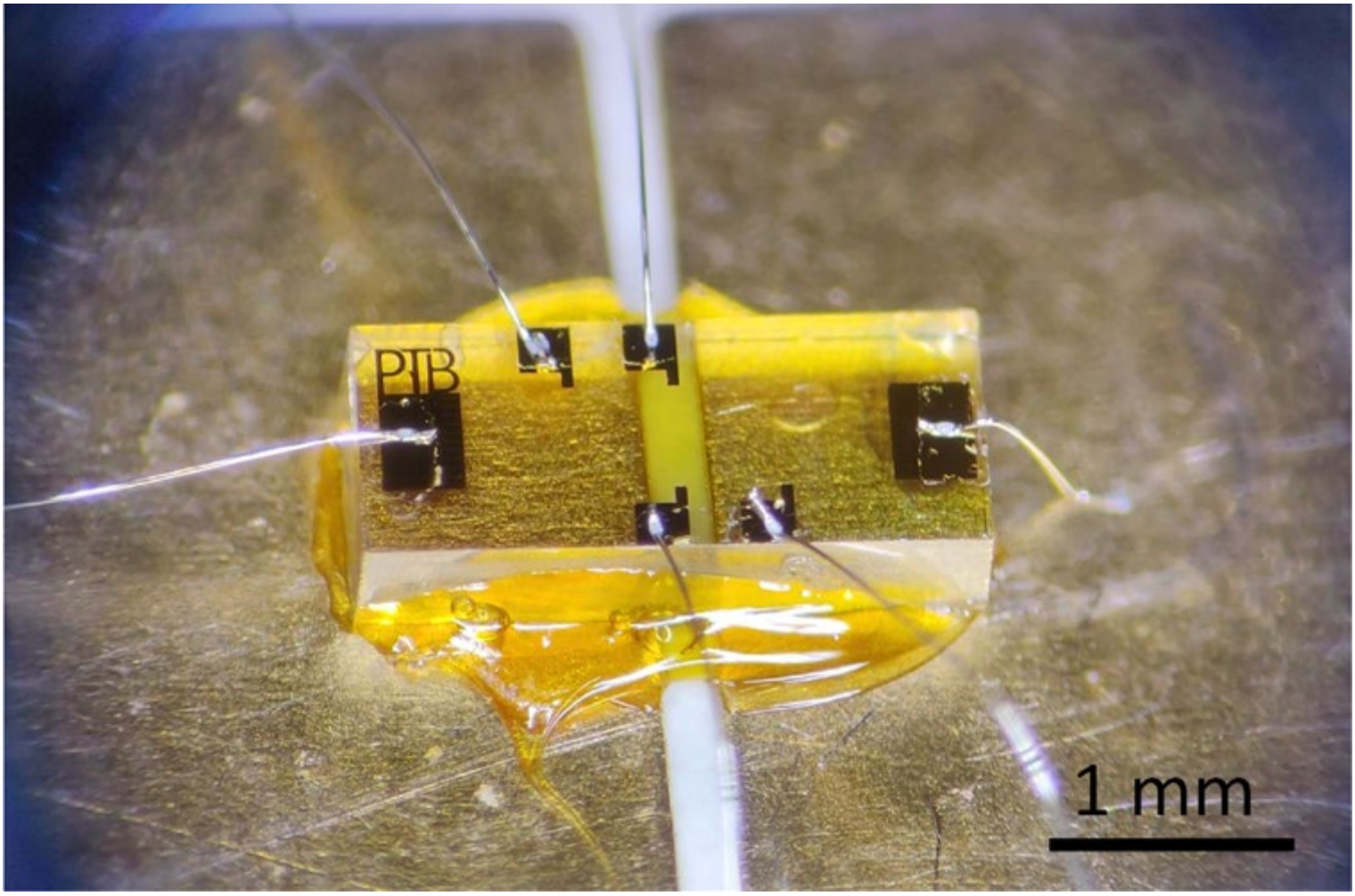


ADVANCED MATERIALS

Tuning graphene for improved electrical systems

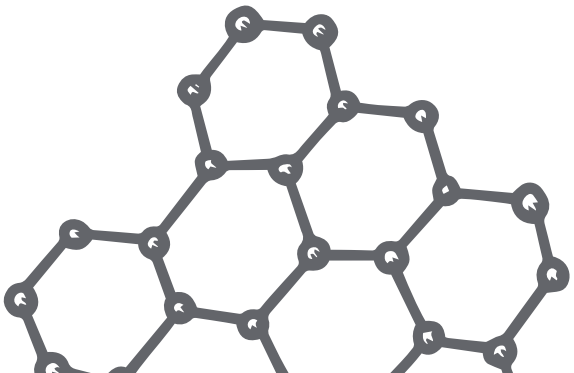
Researchers at the National Metrology Institute (PTB) of Germany investigated the doping behaviour of epitaxial graphene on silicon carbide substrate with a goal to develop a graphene-based quantum standard for electrical impedance. They determined that the surface structure of silicon carbide wafers has a notable impact on the doping state of the 2D-graphene layers.

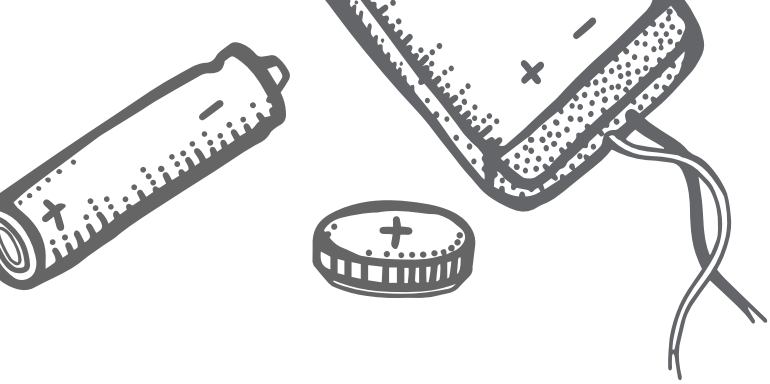
Graphene serves an ideal role for the fabrication of quantum resistance and quantum impedance standards by which the resistance unit ohm and the capacitance unit farad will be realized in the future.

Scientists used X-ray photoemission electron microscopy (XPEEM) at MAXPEEM beamline at MAX IV, among other techniques. The capability to tune graphene-based electrical properties will simplify and improve the calibration of capacitors used with, for example, strain gauges and pressure sensors. Reliable impedance measurements may also improve automotive and mobile electronics in industry.

Publication

D. Momeni Pakdehi, P. Schädlich, T. T. Nhung Nguyen, A. A. Zakharov, S. Wundrack, E. Najafidehaghani, F. Speck, K. Pierz, T. Seyller, C. Tegenkamp, H. Werner Schumacher, Silicon Carbide Stacking-Order-Induced Doping Variation in Epitaxial Graphene, Advanced Functional Materials. 30, 202004695 (2020), DOI: 10.1002/adfm.202004695





ADVANCED MATERIALS

2D MXenes properties hold key to improved energy storage

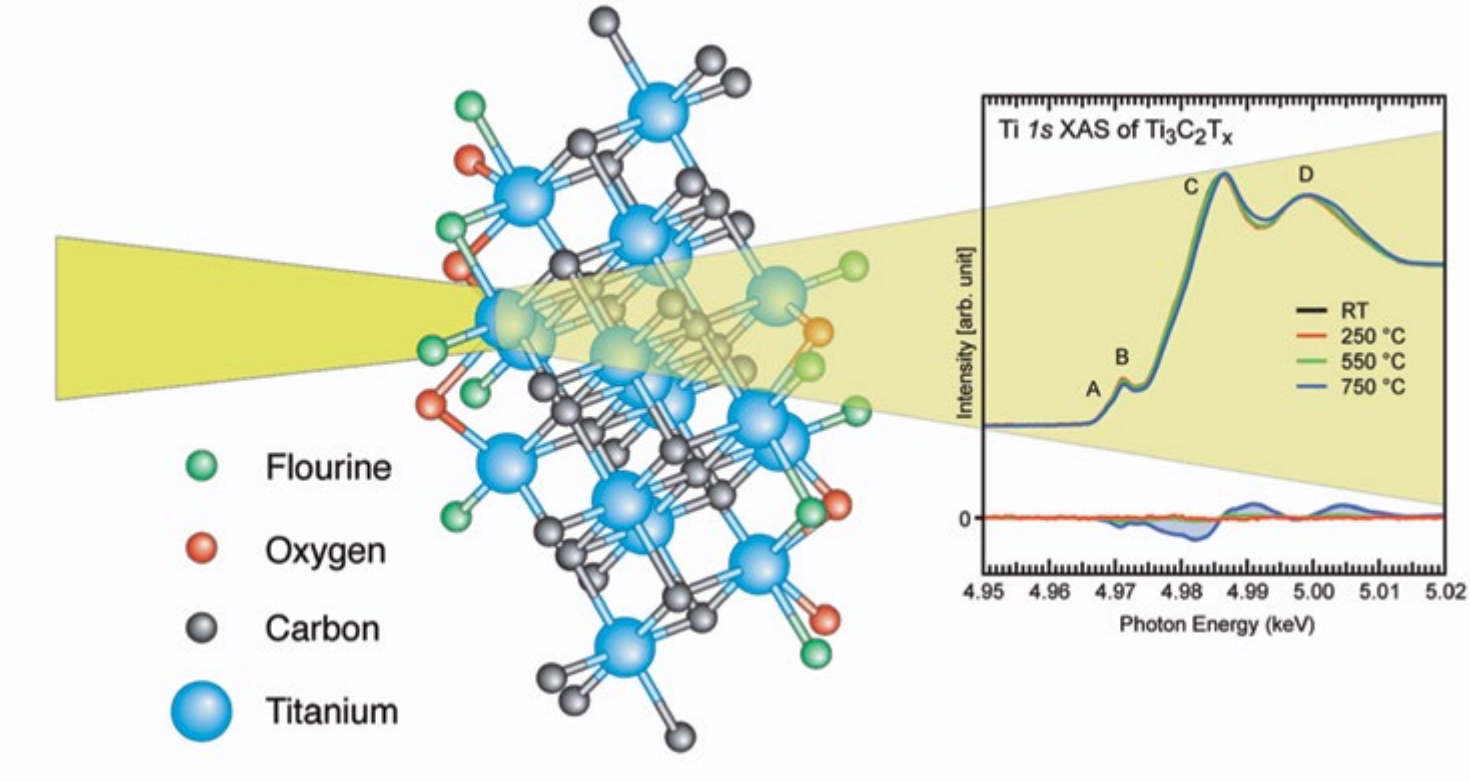
The chemical bonding and structural properties of titanium aluminium carbide MAX phase and 2D titanium carbide MXene were explored by researchers at Linköping University in Sweden. They measured bond lengths between surface titanium atoms and termination species, oxygen and fluorine, respectively, in $Ti_3C_2T_x$ MXene and how surface bonding of the species occurs.

Results showed that the titanium 4p orbital plays a key role due to its sensitivity for the termination species and occupation sites. Utilization of X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS) at MAX IV's Balder beamline resolved the influence of different termination species on the orbital structure.

MXenes are interesting for their surface properties; useful in energy storage applications such as supercapacitors and batteries, and for catalysis and carbon dioxide capture. Knowledge of active orbitals, their configuration on the MXene surface, and of bonding processes, will enable accurate theoretical and experimental structural models.

Publication

M. Magnuson and L. -Å. Näslund, Local chemical bonding and structural properties in Ti_3AlC_2 MAX phase and $Ti_3C_2T_x$ MXene probed by Ti 1s x-ray absorption spectroscopy. Phys. Rev. Research 2, 033516 (2020), DOI: 10.1103/PhysRevResearch.2.033516



ADVANCED MATERIALS

Improving scintillators' efficiency of garnet single crystals

Scintillator detectors are irreplaceable in high-energy physics, spectrometry of low energy γ-quanta, applications in medical imaging, sensors for environmental monitoring, safety systems, space applications, and many more. Among other scintillator materials, GGAG:Ce is one of the most relevant today.

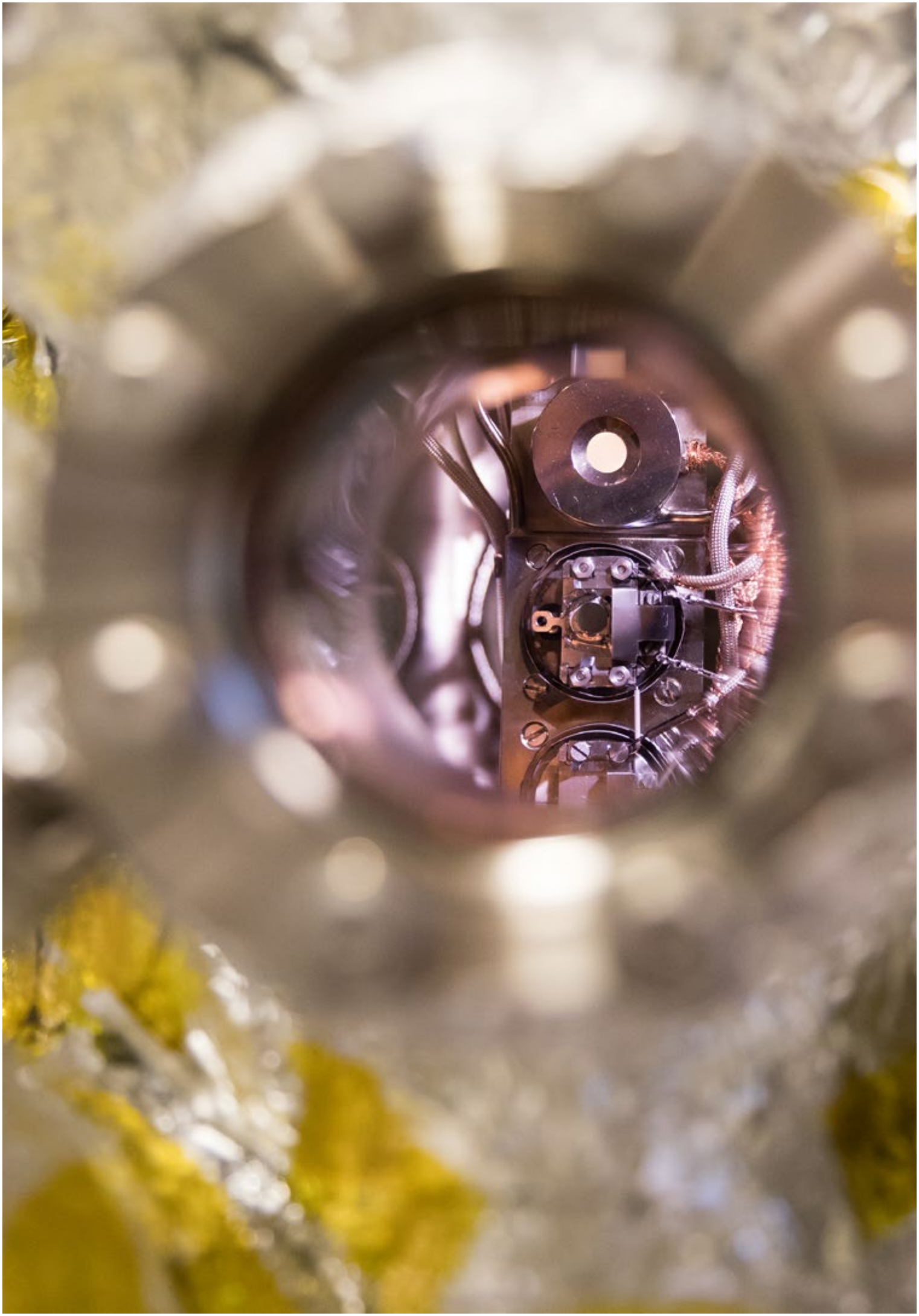
Researchers from the Institute of Solid State Physics University of Latvia investigated the relaxation of electronic excitation processes in GGAG:Ce single crystals to establish the role of defects and impurities in the scintillation mechanisms. The result showed that GGAG:Ce single crystals co-doped by magnesium ions indicated outstanding efficiency of multiplication of electronic excitations in VUV spectral range.

Two models were proposed to explain this phenomenon. First, that co-dopants could influence the thermalization length of geminate electrons and holes. Second, that intrinsic defects in GGAG lattice were responsible for capturing hot charge carriers leading to the degradation of the excitation efficiency in VUV spectral range.

The experiments were carried out at FINEST-LUMI, a specialized FinEstBeAMS' endstation for time-resolved spectroscopic studies of scintillating and luminescent materials.

Publication

A. P. Kozlova, V. M. Kasimovaa, O. A. Buzanov, K. Chernenko, K. Klementiev, V. Pankratov, Luminescence and vacuum ultraviolet excitation spectroscopy of cerium doped $Gd_3Ga_3Al_2O_{12}$ single crystalline scintillators under synchrotron radiation excitations, Results Phys. **16**, 103002 (2020), DOI: 10.1016/j.rinp.2020.103002

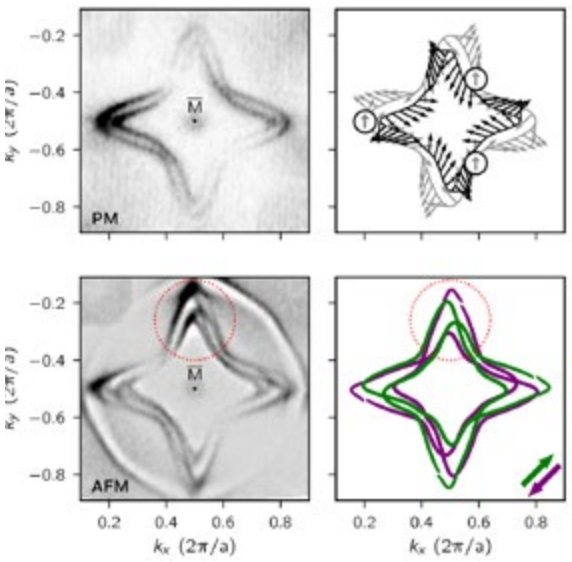


ADVANCED MATERIALS

Exploring Rashba effects and magnetism for spintronic devices

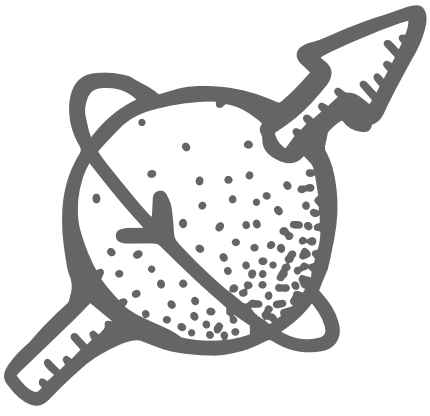
Research led by Donostia International Physics Center (DIPC) in Spain explored the phenomena of Rashba-type spin-orbit coupling effect and its combination with exchange magnetism on the iridium-silicide surface of bulk antiferromagnet, $GdIr_2Si_2$. The researchers detail how the strong spin-orbit coupling in terms of the Rashba-like effects and the exchange interaction between the itinerant surface state electrons and the ordered 4f moments drive the spin polarization of these states.

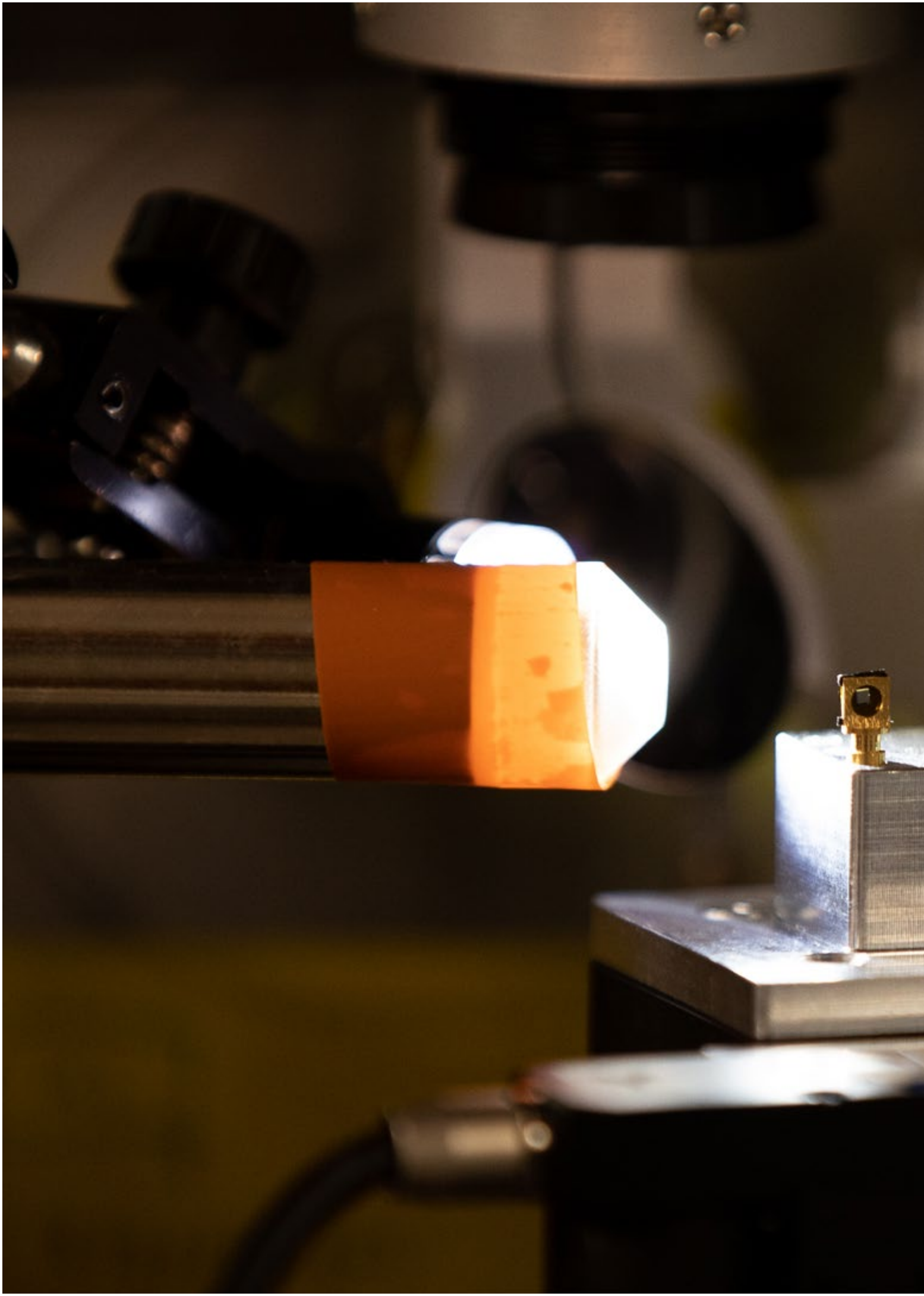
Data from angle-resolved photoemission spectroscopy (ARPES) measurements was generated at Bloch beamline at MAX IV. The study elucidates how the spins of two-dimensional electrons can be manipulated, giving new insights into how Rashba effects can be combined with exchange magnetism for spintronics applications.

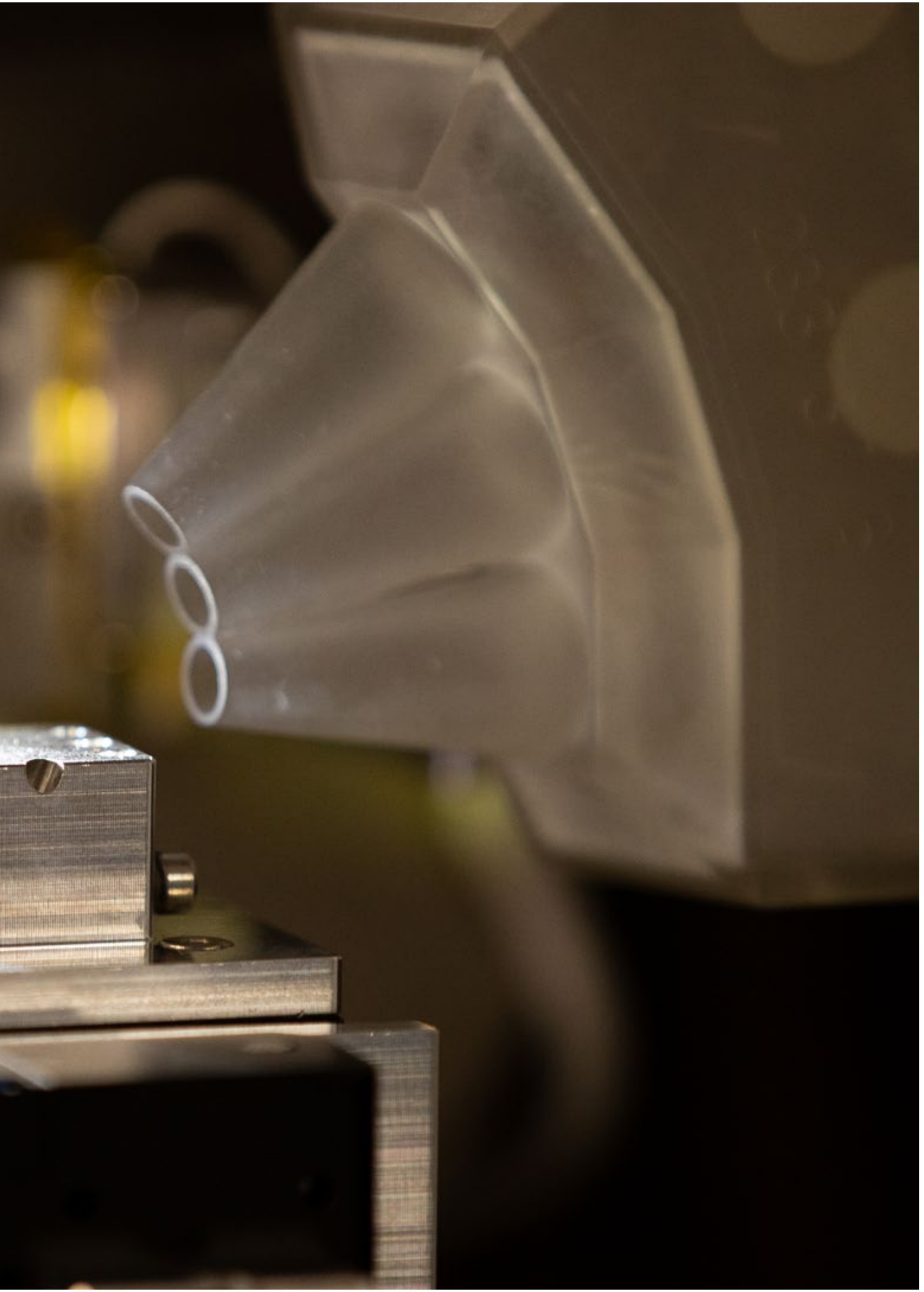


Publication

S. Schulz, A. Yu. Vyazovskaya, G. Poelchen, A. Generalov, M. Güttler, M. Mende, S. Danzenbächer, M. M. Otrokov, T. Balasubramanian, C. Polley, E. V. Chulkov, C. Laubschat, M. Peters, K. Kliemt, C. Krellner, D. Yu. Usachov, and D. V. Vyalikh, Classical and cubic Rashba effect in the presence of in-plane 4f magnetism at the iridium silicide surface of the antiferromagnet $GdIr_2Si_2$. Phys. Rev. B **103**, 035123 (2021), DOI: 10.1103/PhysRevB.103.035123







ENVIRONMETAL SCIENCE

Copper chemistry benefits catalyst development

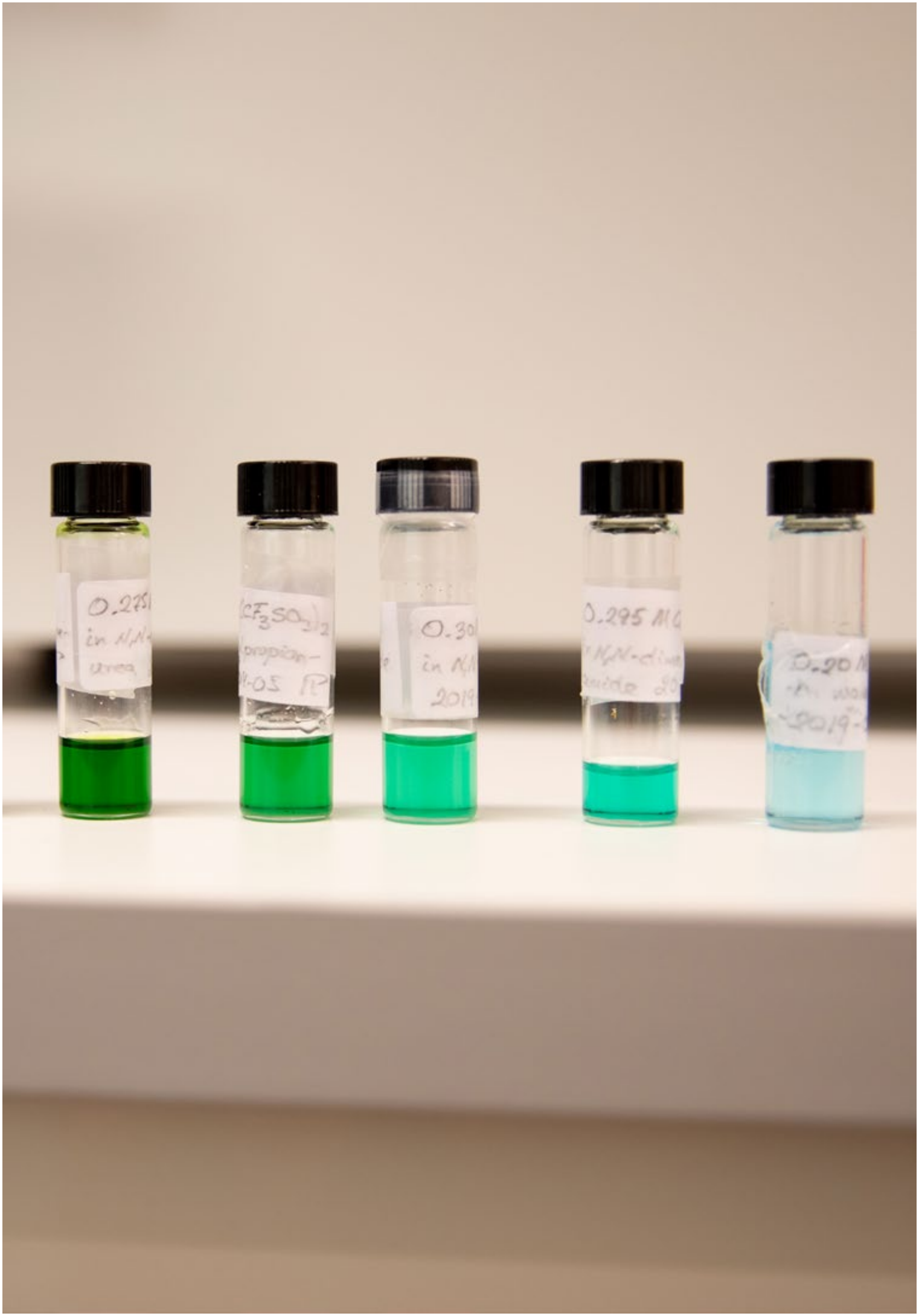
An investigation of copper (II) by the Swedish University of Agricultural Sciences describes the unresolved structure of hydrated copper(II) ion aqueous solution compared to three solid salt compounds with transition metal $[Cu(H_2O)_6]^{2+}$ plus two with water and counter ions binding to copper, and solvated copper (II) ions in nine organic oxygen donor solvents.

Results show that hydrated copper (II) is six-coordinate with non-centrosymmetric tetragonally elongated octahedral geometry. The solvated copper(II) ion is a four-coordinate in square-planar fashion in solvents space-demanding at coordination, and in the seven organic oxygen donor solvents without steric requirements at coordination have the same configuration in solution as the hydrated copper(II) ion.

Measurements were taken with extended X-ray absorption fine structure (EXAFS) technique at Balder beamline at MAX IV. The non-centrosymmetric structure and unique Cu-O bond distances in copper (II) complexes are linked with copper reactivity. Greater understanding can open new paths to develop technical and biological applications such as catalysts.

Publication

I. Persson, D. Lundberg, É. G. Bajnóczi, K. Klementiev, J. Just, and K. G. V. Sigfridsson Clauss, EXAFS Study on the Coordination Chemistry of the Solvated Copper(II) Ion in a Series of Oxygen Donor Solvents. Inorg. Chem. **59**, 9538 (2020), DOI: 10.1021/acs.inorgchem.0c00403



ENVIRONMENTAL SCIENCE

Recycled waste ash for building material

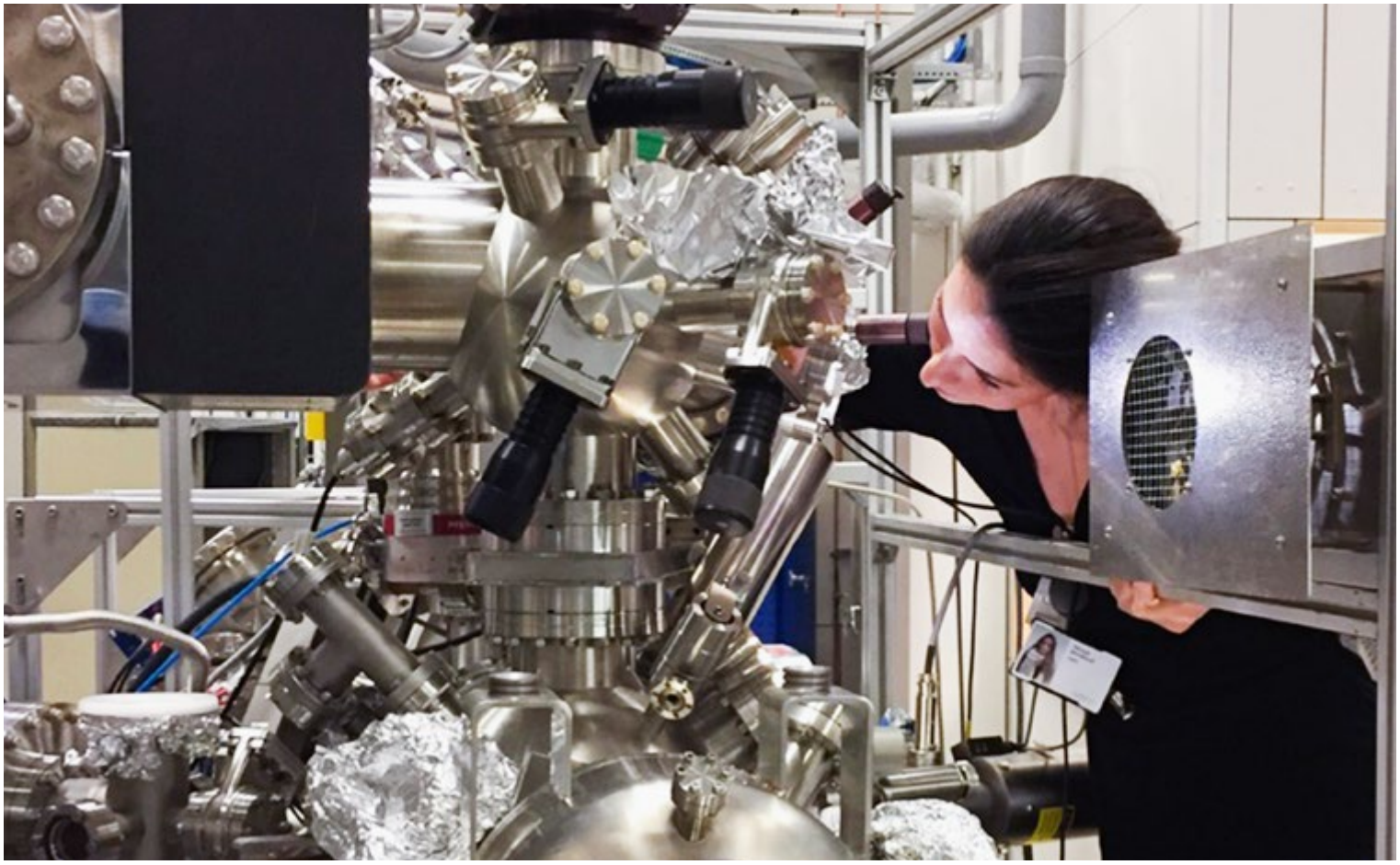
Researchers at RISE Research Institutes of Sweden and Chalmers University of Technology in Sweden examined the chemical forms of trace metals, zinc, copper, and lead, in ash from waste incineration. Identifying the levels and chemical species of heavy metals or ecotoxicity in fly and bottom ash may enable use of ash as a secondary source of salts and metals or as ground construction materials.

Ash from three different waste incinerator facilities was analysed at MAX IV's Balder beamline with X-ray absorption spectroscopy (XAS) and X-ray absorption near edge structure (XANES) techniques. Results showed the various oxidation states of the metals, with several chemical forms occurring in the same samples and up to eight different forms present. A library of reference compounds was developed for future determination of ash chemical species.

The potential safe use of ash offers an alternative to finite virgin materials and provides a circular economic incentive for society.

Publication

J. Rissler, K. Klementiev, J. Dahl, B. -M. Steenari, and M. Edo, Identification and Quantification of Chemical Forms of Cu and Zn in MSWI Ashes Using XANES. Energy Fuels 34, 14505 (2020), DOI: 10.1021/acs.energyfuels.0c02226



ENVIRONMENTAL SCIENCE

Reactive particle surfaces could prompt revision of climate models

Aerosol particles in the atmosphere play important roles in atmospheric chemistry, the formation of air pollution, and our climate. Chemical and physical reactions on the surfaces of the aerosol particles are critical for each of these effects. For example, reactions that release halogens from aerosol particles is a key part of the ozone cycle.

A study led by researchers from the ATMOS centre at the University of Oulu revealed surprising molecular-level information about water uptake to aerosol particle surfaces. Water is taken up already at humidities corresponding to some of the driest conditions in the troposphere and leads to chemical changes in the surface layer of the particles.

The surface reactions could affect how particles contribute to transforming the atmosphere and how they influence the climate system, potentially warranting a need to revise models. The experiments were conducted using surface-sensitive Ambient Pressure X-ray Photoelectron Spectroscopy at the SPECIES beamline.

Publication

J. J. Lin, R. R. Kamal, S. Wang, E. Kokkonen, M. -H. Mikkelä, S. Urpelainen, and N. L. Prisle, Pre-deliquescent water uptake in deposited nanoparticles observed with in situ ambient pressure X-ray photoelectron spectroscopy, Atmos. Chem. Phys. **21**, 4709 (2020), DOI: 10.5194/acp-21-4709-2021

CATALYSIS

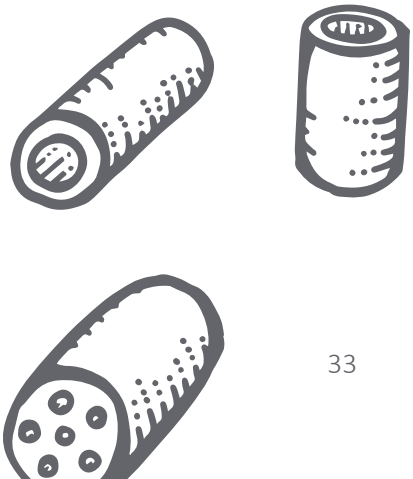
The role of synthesis gas in tomorrow's sustainable fuels

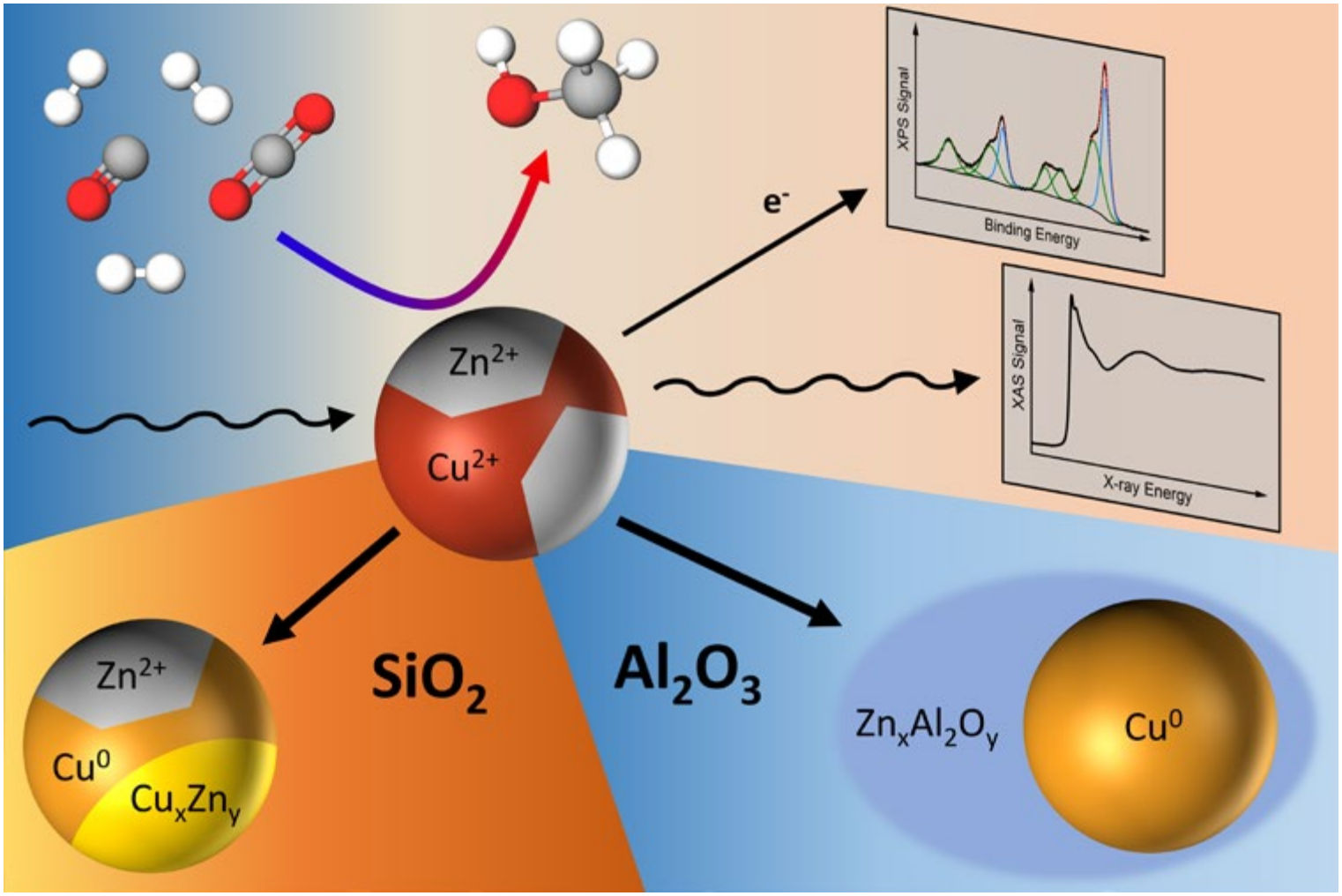
Today the synthesis gas, CO and H_2, used to produce synthetic oil by Fischer-Trospch synthesis comes from fossil sources. Via better molecular-scale understanding, the process could be more sustainable with CO_2 from biomass and H_2 from water. In a study led by scientists from Syngaschem, the Netherlands, the molecules present in the industrial process were observed on a model cobalt catalyst surface.

The research team show that CO and H strongly influence reactions of hydrocarbon surface species, contributing to a more efficient carbon-carbon bond forming reaction. CO is needed as a reactant and, at the same time, also acts as a promoter to steer the reaction towards long hydrocarbon chains. The research team used X-ray photoelectron spectroscopy (XPS) at beamline HIPPIE to identify the chemical species present on the surface during the reaction at ultra-high vacuum and near ambient conditions.

Publication

C. J. Weststrate, D. Sharma, D. G. Rodriguez, M. A. Gleeson, H. O. A. Fredriksson & J. W. Niemantsverdriet, Mechanistic insight into carbon-carbon bond formation on cobalt under simulated Fischer-Tropsch synthesis conditions, Nat. Commun. 11, 750 (2020), DOI: 10.1038/s41467-020-14613-5





CATALYSIS

Zinc oxide interaction important for methanol synthesis

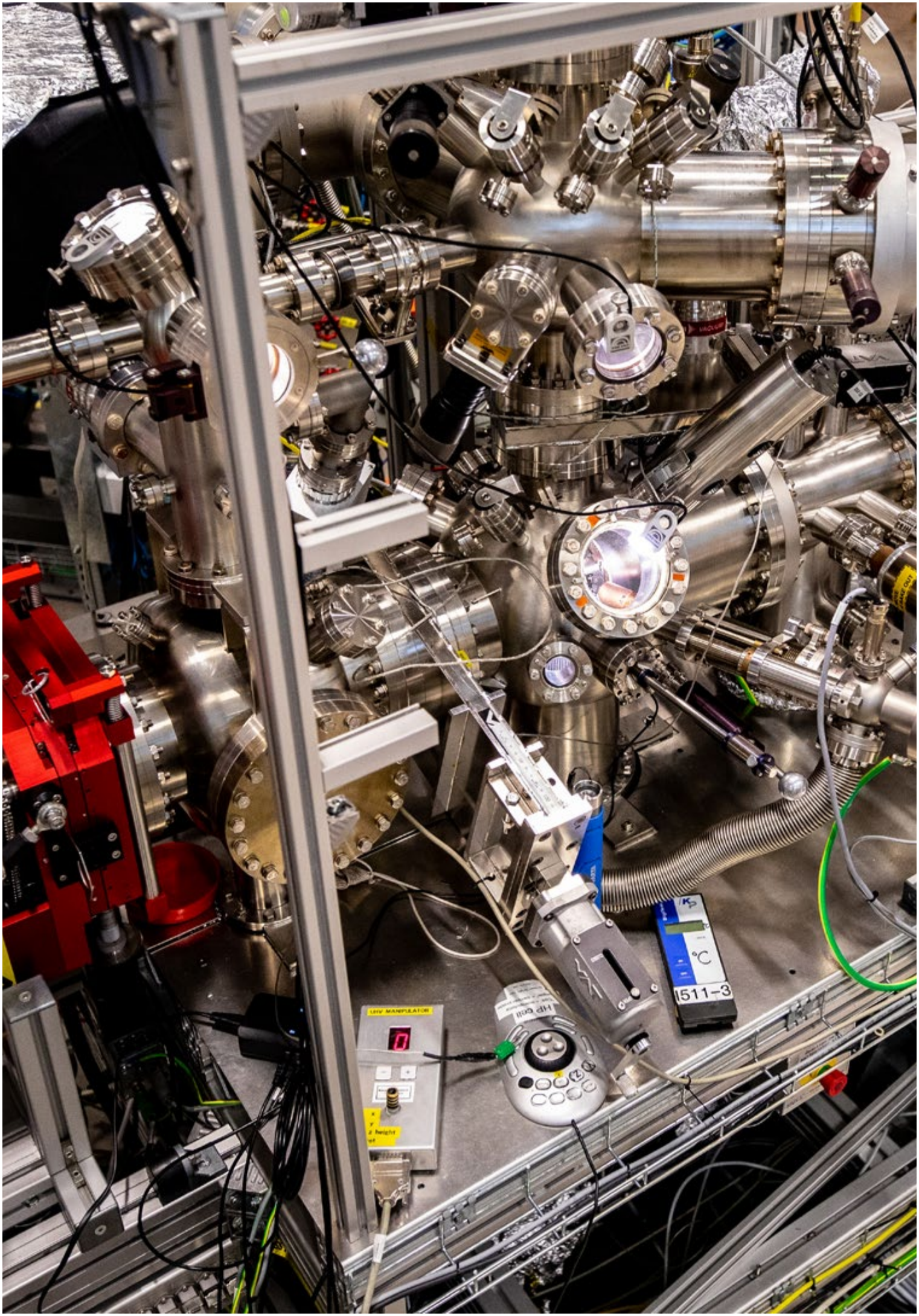
A team of researchers led by scientists from the Fritz Haber Institute has shown that minute amounts of ZnO present in Cu/ZnO catalysts for the conversion of synthesis gas into methanol are essential for an efficient reaction. In addition, the choice of support material for the catalyst is important for the nanoparticle-support interaction, especially for the Zn component, and can improve its longevity.

The study's goal was to improve future catalysts by understanding changes in activity and selectivity on a molecular scale. The researchers used operando Ambient Pressure X-ray Photoelectron Spectroscopy to investigate the restructuring of the nanoparticles under reaction conditions.

Understanding catalysis for methanol production is essential as it acts as a raw material for many necessary chemicals. The process can also convert the greenhouse gas CO2, which is present in synthesis gas, into something useful.

Publication

N. J. Divins, D. Kordus, J. Timoshenko, I. Sinev, I. Zegkinoglou, A. Bergmann, S. W. Chee, S. Widrinna, O. Karslıoğlu, H. Mistry, M. L. Luna, J. Qiang Zhong, A. S. Hoffman, A. Boubnov, J. Anibal Boscoboinik, M. Heggen, R. E. Dunin-Borkowski, S. R. Bare, and B. Roldan Cuenya, Operando high-pressure investigation of size-controlled CuZn catalysts for the methanol synthesis reaction, Nat. Commun. **12**, 1435 (2021), DOI: 10.1038/s41467-021-21604-7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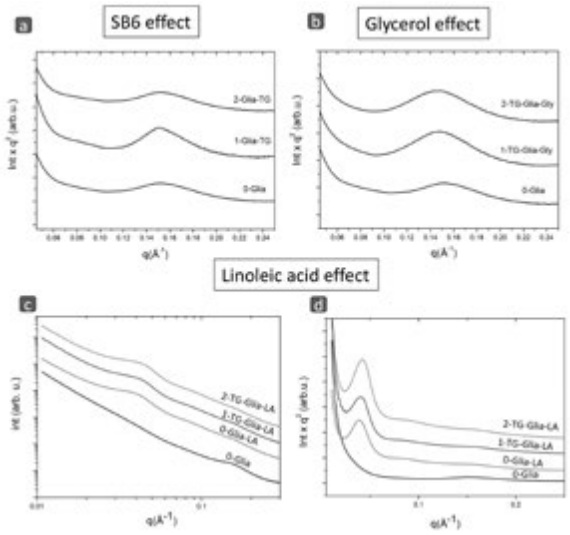
FOOD

Unlocking intriguing morphologies in plant protein porous foods

The rise of awareness of plant-based protein and protein-enriched foods prompts the search for locally sourced animal proteins alternatives and potential soy substitutes. To address this need and explore innovative functionalities of locally grown crops in food applications, researchers from the Plant Product Quality group at SLU, Alnarp, Sweden, discovered new insights on the impact of food additives in the development of solid edible gliadin foams and their unique structural and functional properties.

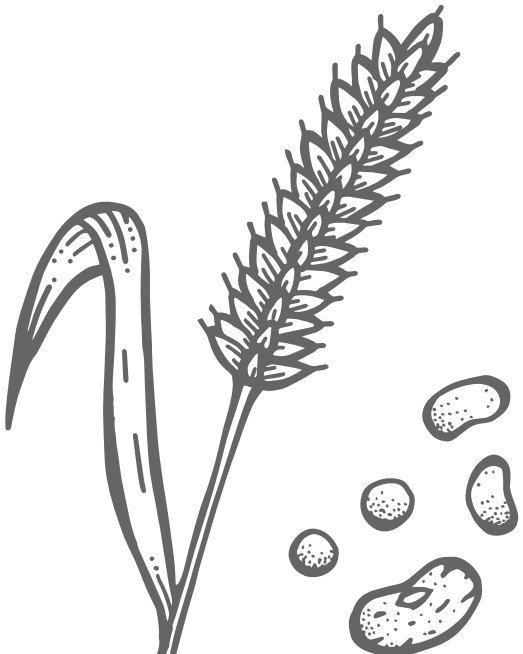


High transglutaminase concentration contributed to the larger sizes of gliadin bubbles and their spatial homogeneity. Bubble sizes imparted differences in textural and morphological aspects of gliadin protein foods. At the same time, the addition of transglutaminase and glycerol transformed the bubble sizes and texture into a more compact look.

Nanomorphology studied by SAXS indicated that glycerol imparted the unfolding of gliadin, while linoleic acid contributed to the formation of lamellar phases in the gliadin foams. This study highlighted few crucial aspects that steer the construction of gliadin protein food structures and brought more knowledge on the impact of various food additives in plant protein-rich products.

Publication

E. Berger Ceresino, E. Johansson, H. Harumi Sato, T. S.Plivelic, S. A.Hall, R. Kuktaite, Morphological and structural heterogeneity of solid gliadin food foams modified with transglutaminase and food grade dispersants. Food Hydrocolloids, Volume **108**, 105995 (2020), DOI: 10.1016/j.foodhyd.2020.105995



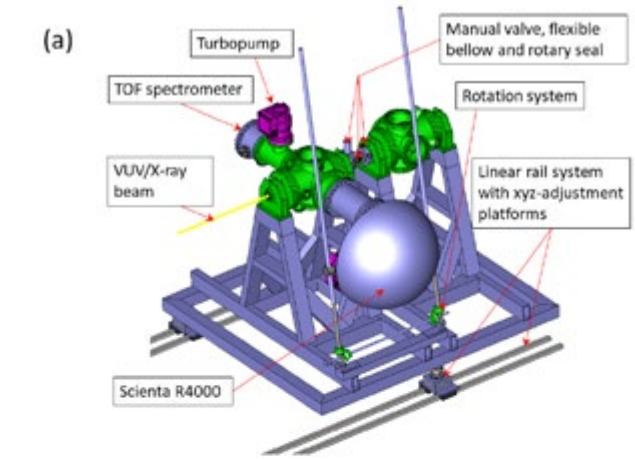
INSTRUMENTATION

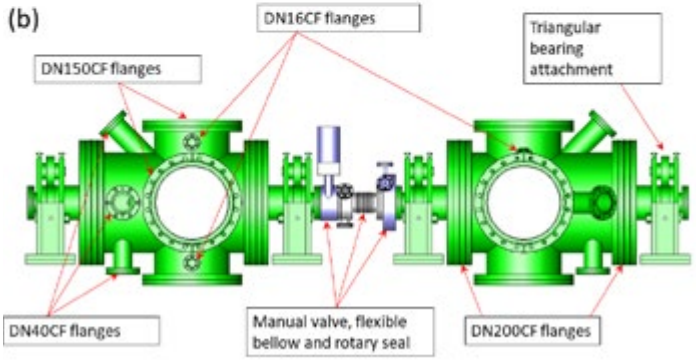
Shining the lights on molecular reaction dynamics

Molecular photo fragmentation is one of the essential branches of studies concerning molecular reaction dynamics. This prompted researchers from Finnish (Turku, Oulu, Tampere) and Estonian (Tartu) universities to develop the gas-phase endstation meant for spectroscopic studies of diluted gas phase samples like molecules, (micro)clusters, free-standing nanoparticles as well as liquids at the FinEstBeAMS beamline.

Its high-resolution electron spectrometer and momentum-resolving, multi-coincidence ion time-of-flight mass spectrometer allow for multi-faceted study of the photoinduced processes. When operating in the electron-ion coincidence mode, the endstation is optimized to characterize the photoinduced dynamics in small quantum systems as thoroughly as possible. Early experiments on ammonia and thiophene demonstrated the suitability and versatility of the endstation's coincidence measurement capabilities.

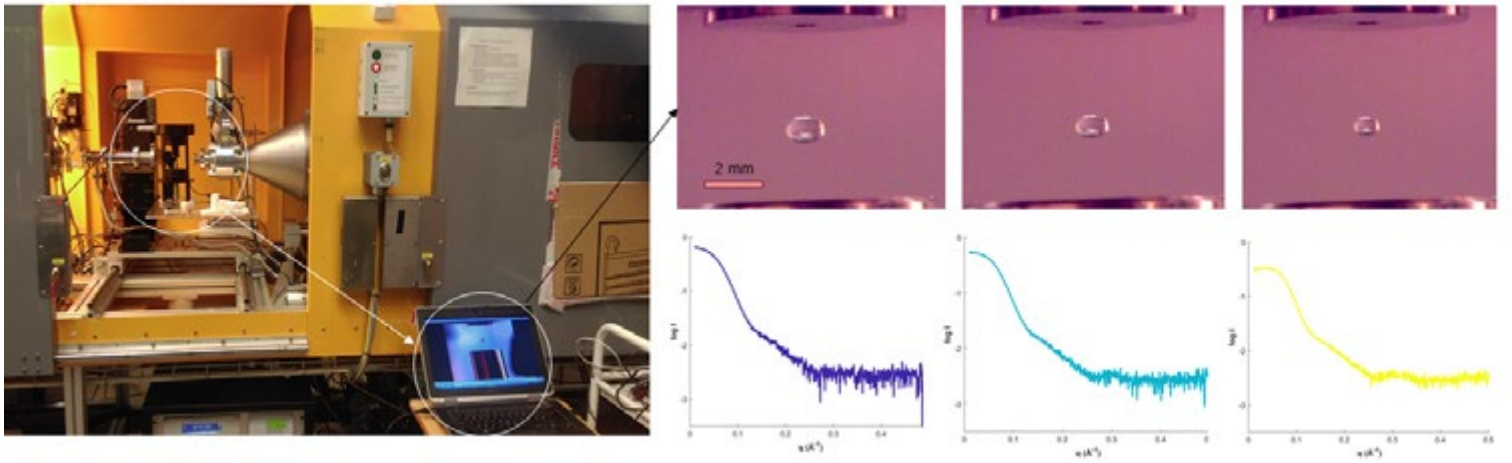
The setup also demonstrated the possibility to compare the electron spectroscopic results of diluted samples with the solid targets in the case of Co2O3 and Fe2O3 at the Co, Fe L2,3-absorption edges. Research on atmospheric science, combustion, and electrochemical processes, among others, will benefit from this setup.





Publication

K. Kooser, A. Kivimäki, P. Turunen, R. Pärna, L. Reisberg, M. Kirm, M. Valden, M. Huttula and E. Kukk, Gas-phase endstation of electron, ion and coincidence spectroscopies for diluted samples at the FinEstBeAMS beamline of the MAX IV 1.5 GeV storage ring. J. Synchrotron Rad (2020), 27, 1090-1091. DOI: 10.1107/S1600577520007146



INSTRUMENTATION

Levitating protein solution studied by SAXS

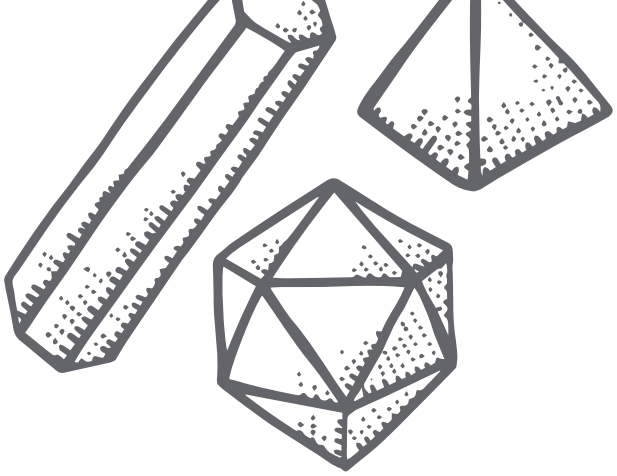
A collaboration between the SAXS group at MAX-IV and a team from the University of Copenhagen (previously at DTU Chemistry) resulted in an innovative methodology to improve data collection, data analysis, and maps correlation with potential interest to both academia and the biopharmaceutical industry in areas of drug discovery, delivery, and production.

By using an acoustically levitated solution mounted on the I911-4 SAXS beamline, the new method allows the study of high-concentrated protein solutions starting with very low sample volumes (lower than 3 mL). Highly concentrated samples (>100g/L) characterization is very relevant as most drugs are administered in high concentrations.

The setup has extra additions compared with standard flow-through cells since it avoids non-desirable interactions between the protein and the sample holder walls and reduces the radiation damage introduced by the X-rays.

Publication

I. Kamenskikh, E. Tishchenko M. Kirm, S. Omelkov, A. Belsky, and A. Vasil'ev, Concentrated protein solutions investigated using acoustic levitation and small-angle X-ray scattering. J. Synchrotron Rad. 27, 396 (2020), DOI: 10.1107/S1600577519016977



INSTRUMENTATION

Decoding the dancing nanoparticles

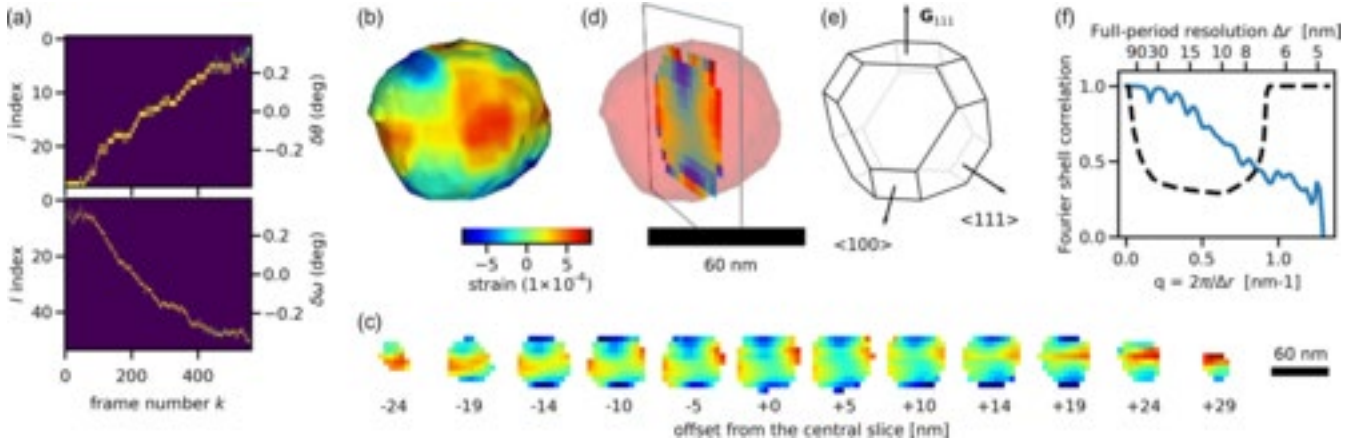
In studying nanoparticles, the imaging technique BCDI (Bragg coherent diffraction imaging) has challenges with smaller nanoparticles: they are more likely to move around unpredictably due to the radiation. When studying catalysis in an electrochemical setting, researchers from MAX IV, University of Uppsala, University of Alicante, and SLJUS Lund, developed a solution to this problem.

They created and validated an adapted diffraction volume assembly algorithm that exploited the uncontrolled rotation induced by the beams to obtain 3D shapes and strain fields of an unstable nanoparticles: gold.

The researchers used NanoMAX's diffraction end station that focuses X-rays down to a spot of 100x100 nanometer and a robot-mounted detector. Detailed understanding of how small nanoparticles catalyze such reactions laid the groundwork for better catalyst design for technology applications in energy conversion, water treatment, etc.

Publication

Alexander Björling, Lucas A. B. Marçal, José Solla-Gullón, Jesper Wallentin, Dina Carbone, and Filipe R. N. C. Maia, Three-Dimensional Coherent Bragg Imaging of Rotating Nanoparticles. Phys. Rev. Lett. 125, 246101 (2020). DOI: https://doi.org/10.1103/PhysRevLett.125.246101



INSTRUMENTATION

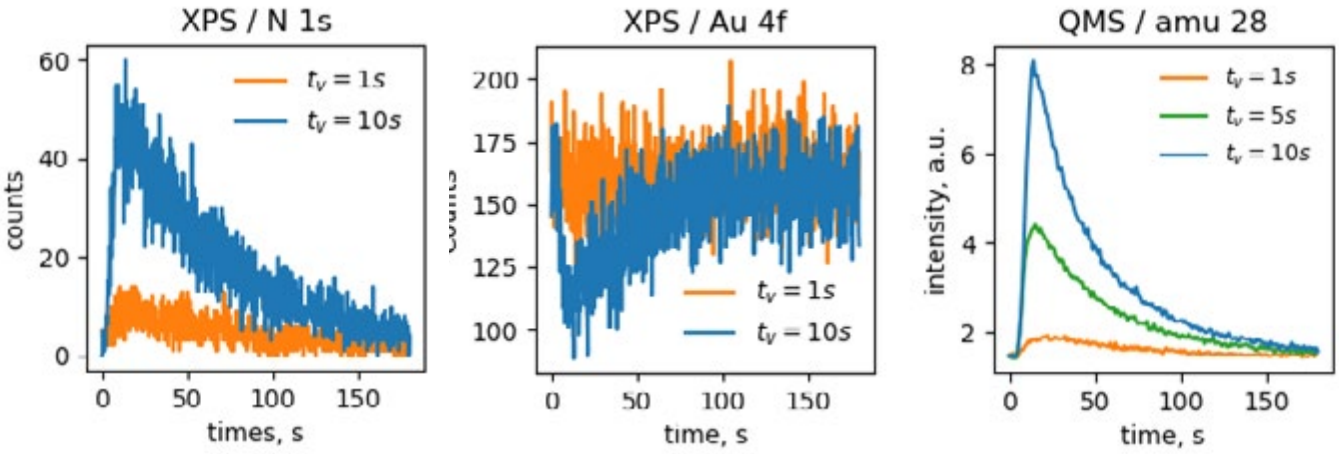
Combination of methods reveals dynamic gas reactions on materials surfaces

Ambient Pressure X-Ray Photoelectron Spectroscopy (APXPS) provides unique information on gas-solid chemical reactions by allowing for higher reactant pressures than in an ordinary X-ray Photoelectron Spectroscopy (XPS) experiment. However, APXPS experiments are typically conducted under conditions where access is limited to detailed time-resolved information about the kinetics of chemical reactions on surfaces of materials.

A team led by researchers from the University of Oslo have, therefore, implemented a novel hardware/software interface for time-resolved APXPS experiments. The interface includes additional electronics and gas handling components inspired by Temporal Analysis of Products (TAP). The techniques are combined to derive complementary spectroscopic and kinetic data about complex reaction mechanisms at surfaces. The researchers used the APXPS setup at beamline SPECIES to test the method. Examples of areas that benefit from the outcome are performance studies of catalytic materials, production of nanomaterials and thin-films as well as corrosion studies or aerosol surfaces in atmospheric research.

Publication

E. A. Redekop, N. Johansson, E. Kokkonen, S. Urpelainen, F. Lopes da Silva, M. Kaipio, H. -E. Nieminen, F. Rehman, V. Miikkulainen, M. Ritala, and Unni Olsbye, Synchronizing gas injections and time-resolved data acquisition for perturbation-enhanced APXPS experiments, Rev. Sci. Instrum. **92**, 044101 (2021), DOI: 10.1063/5.0039957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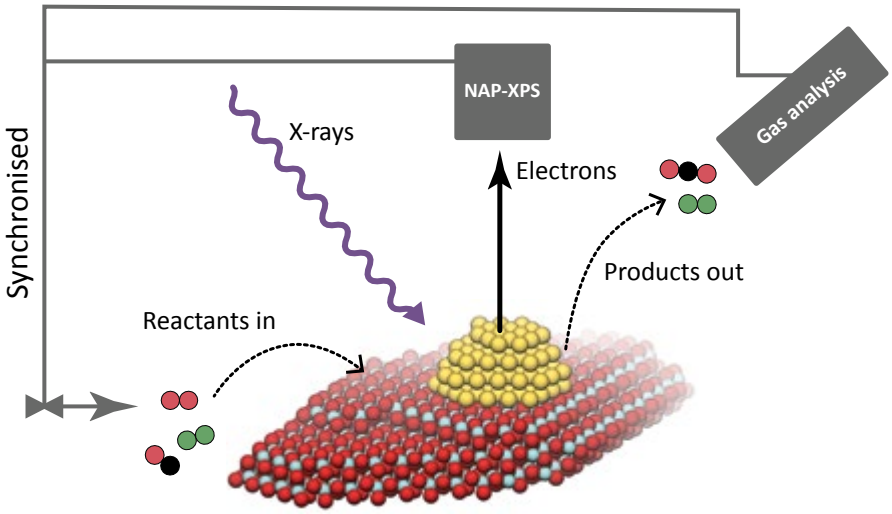
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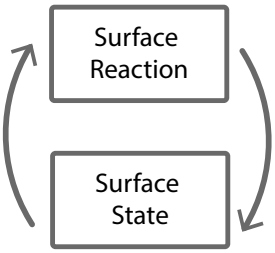
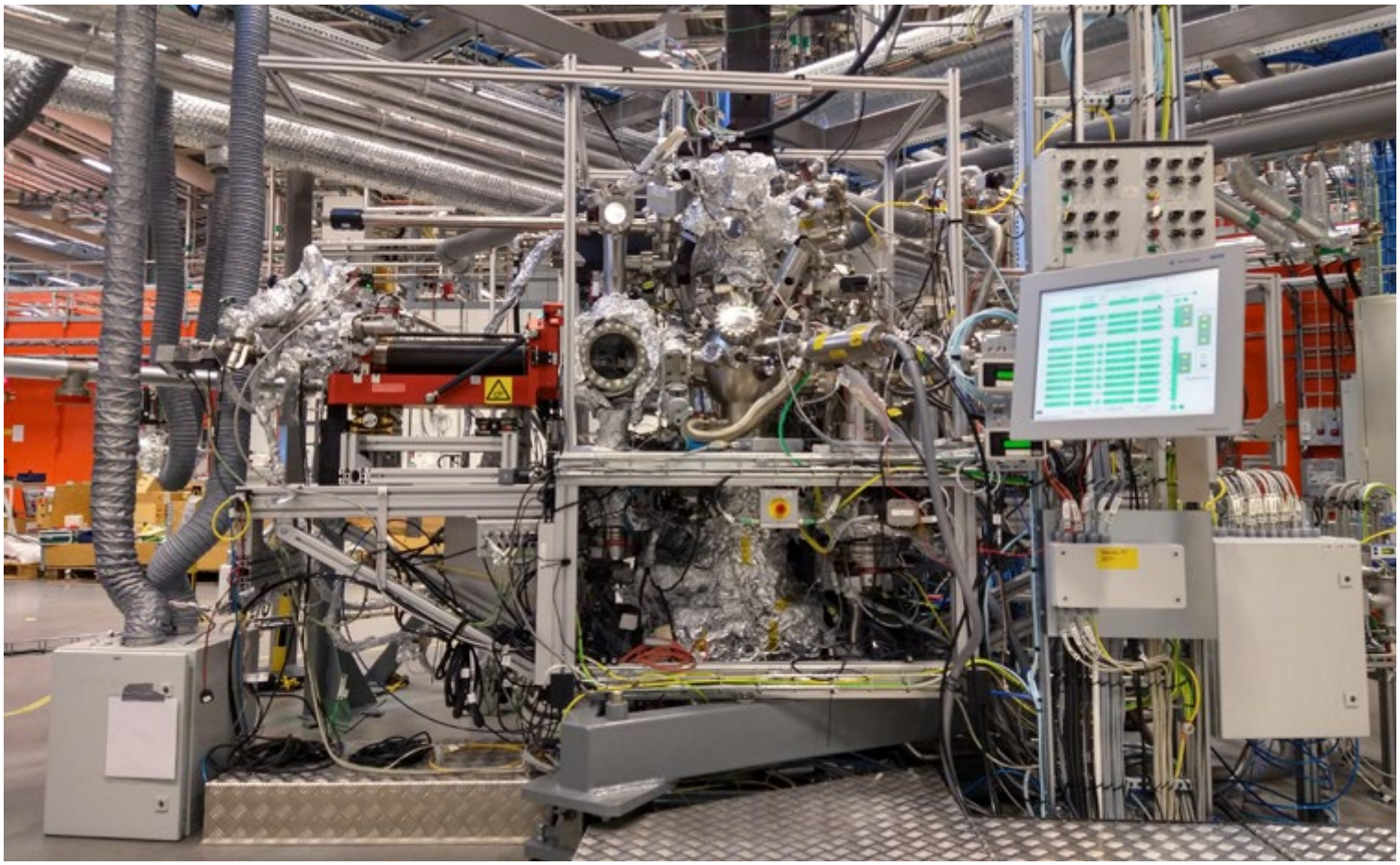
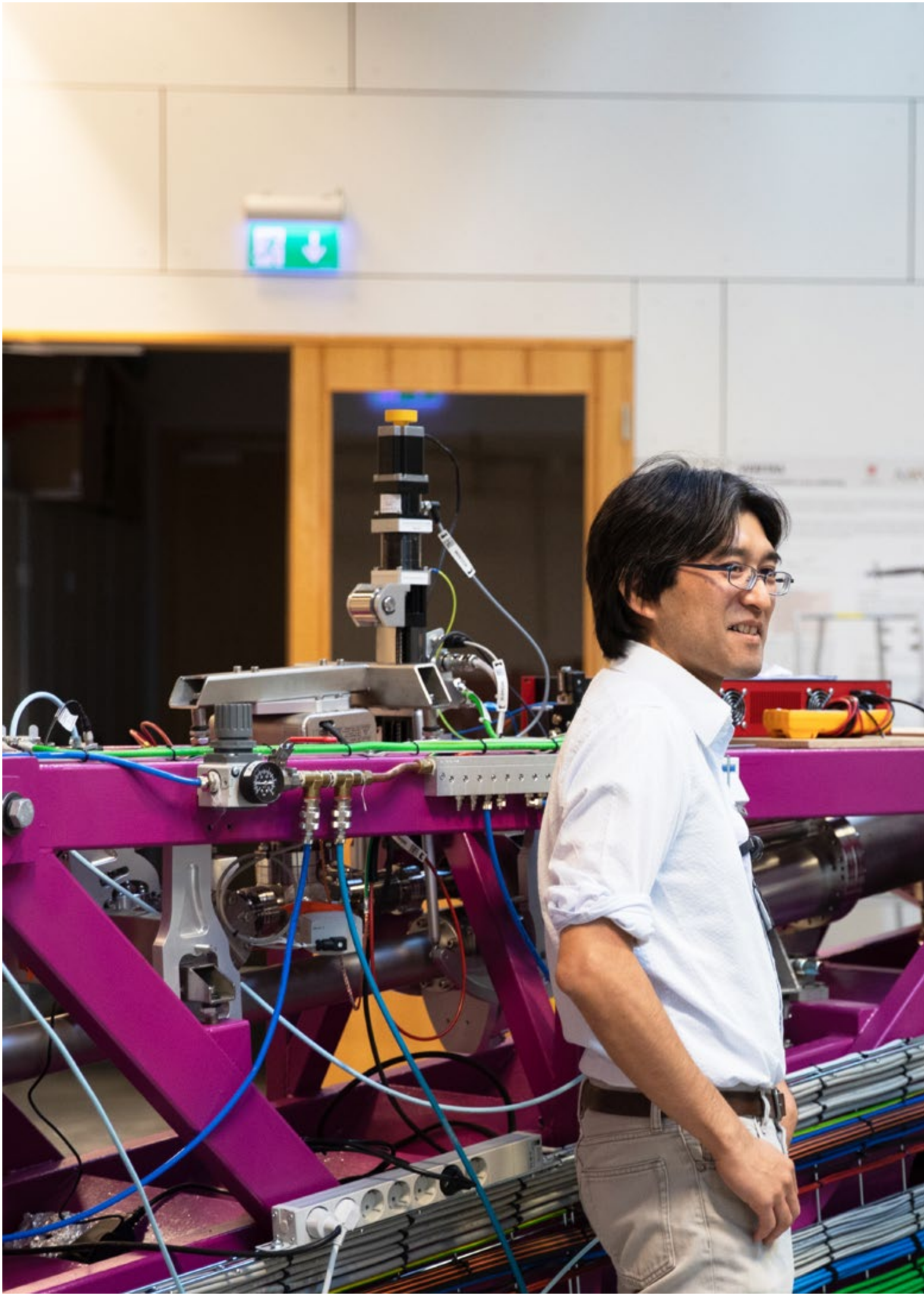
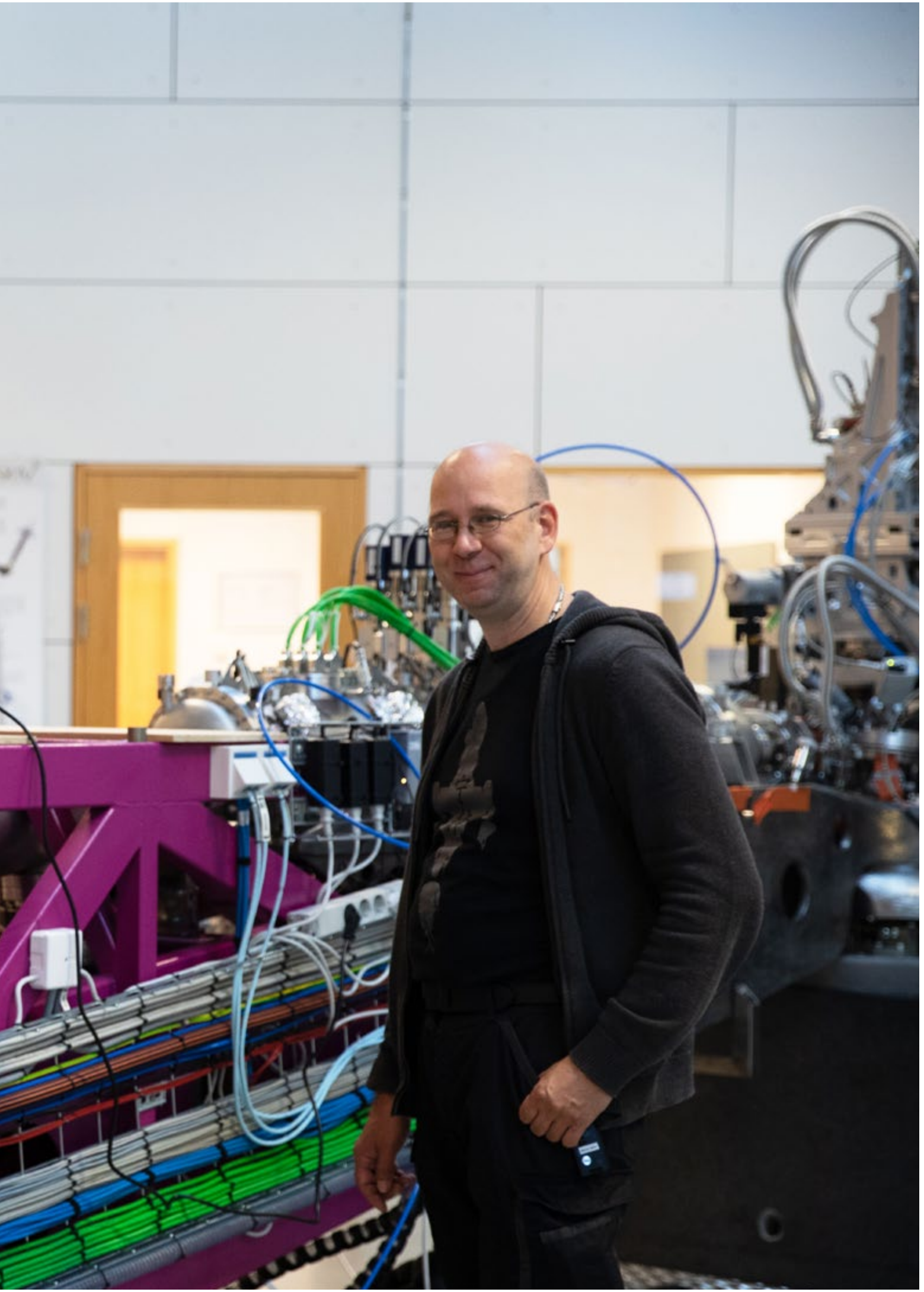
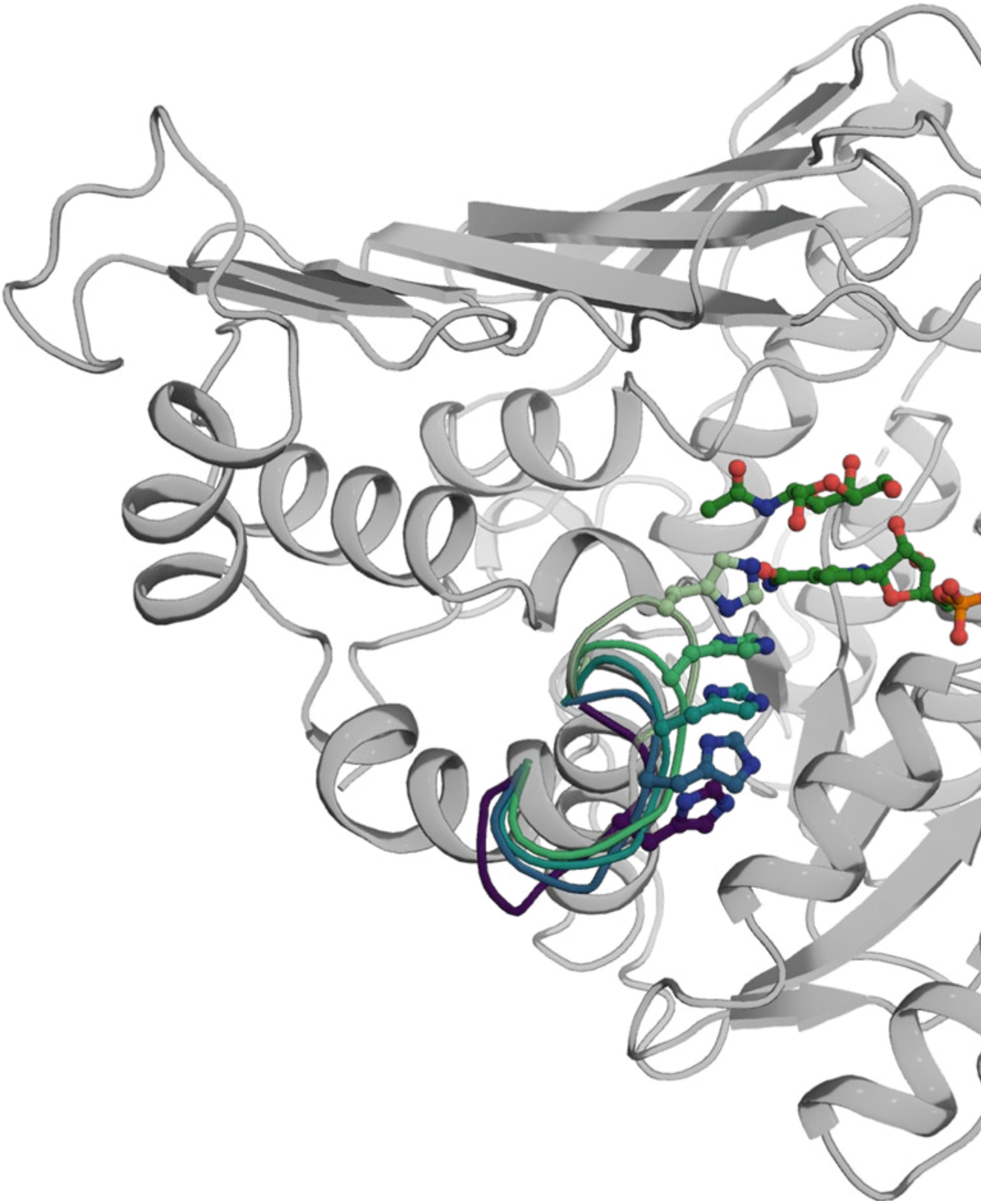
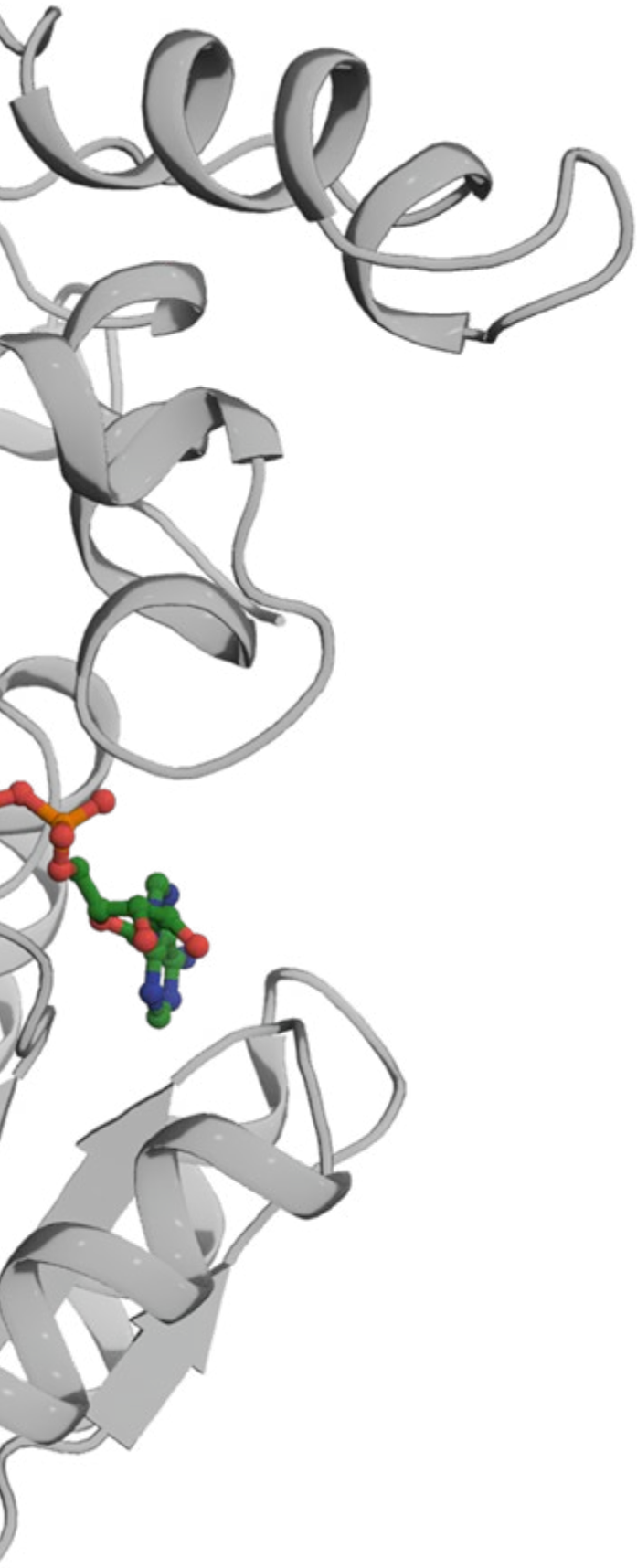

Surface Reaction
Surface State











HEALTH AND MEDICINE

Gut microbial activity probed for better health

Scientists proposed the full catalytic machinery in a large family of NAD-dependent glycoside hydrolases associated with metabolism of host-derived glycans in the human gut. This was possible with the identification of a previously unknown catalytic base in an enzyme encoded by bacterium symbiont A. muciniphila. The symbiont is associated with structural integrity of the gut barrier and homeostatis of the mucosa layer which protects against microbial and physical damage.

The research was led by the Abou Hachem laboratory at the Technical University of Denmark (DTU), with X-ray measurements taken at BioMAX beamline at MAX IV. The study provides a framework for function-based understanding of the role of key mucin adherent gut microbiota, and potential for applications in biotechnology or glycobiology. Insight into enzyme activity and machinery may promote better gut health and help combat inflammatory bowel diseases and colorectal cancer.

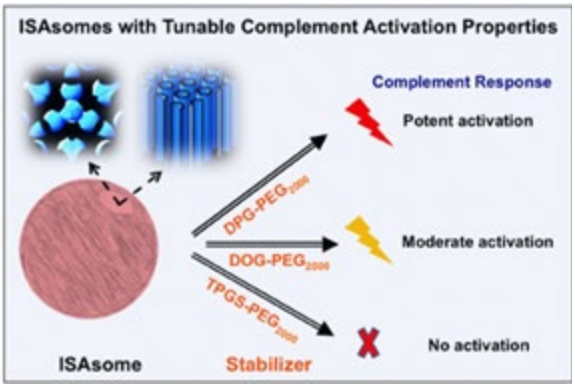
Publication

D. Teze et al, The Catalytic Acid–Base in GH109 Resides in a Conserved GGHGG Loop and Allows for Comparable α-Retaining and β-Inverting Activity in an N-Acetylgalactosaminidase from Akkermansia muciniphila. ACS Catal. 2020, 10, 6, 3809–3819. DOI: 10.1021/acscatal.9b04474

HEALTH AND MEDICINE

Innovative non-lamellar LLC nano-self-assemblies as safer drug nanocarriers

Non-lamellar liquid crystalline (LLC) nanodispersions, including cubosomes and hexosomes, are attractive in the development of nanocarriers for drug delivery applications. However, most investigated nanoparticulate formulations stabilized with Pluronic F127 (a well-known triblock copolymer) are not safe and potent activators of the human complement system. This may lead to inflammatory reactions, depending on dose and route of administration.

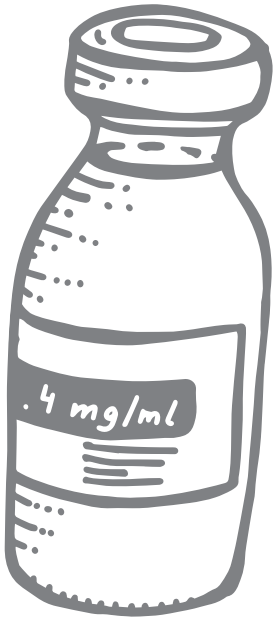


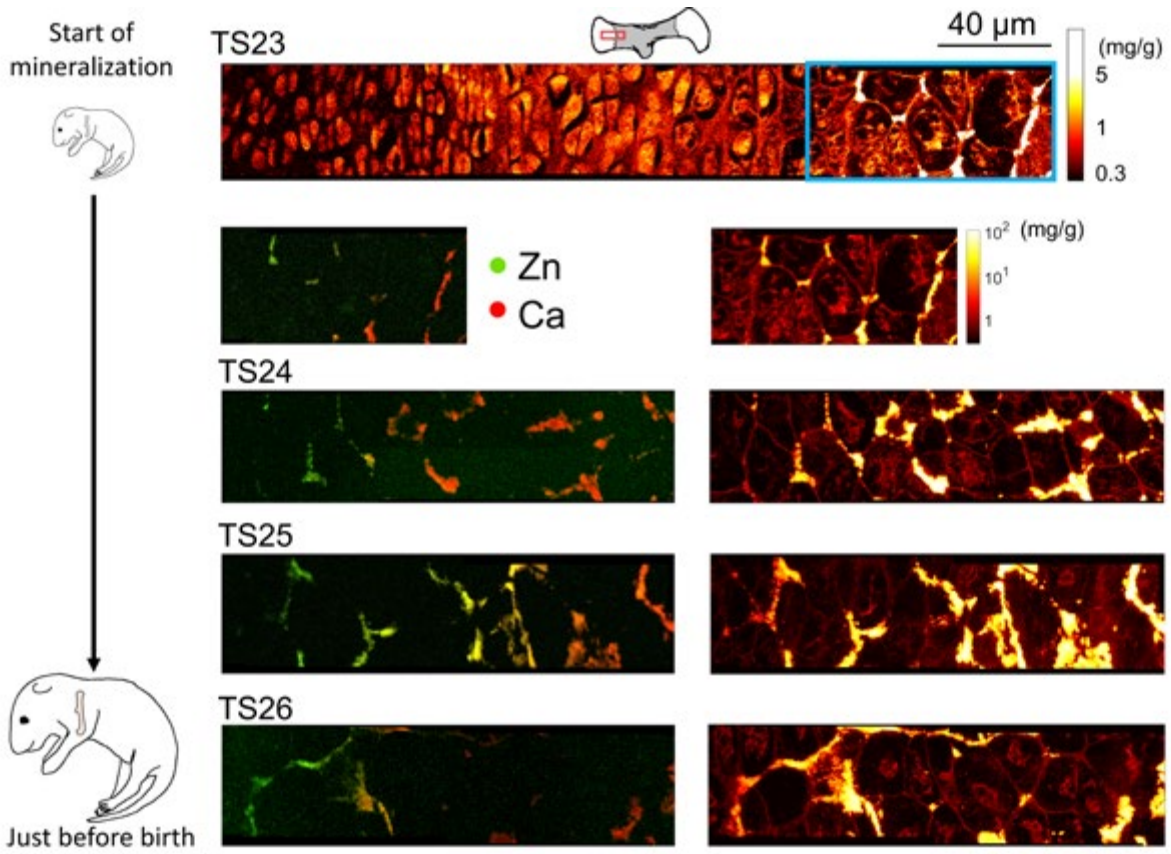
An innovative research between the University of Copenhagen and Newcastle University introduced a broad family of LLC nanodispersions from glycerol monooleate (GMO) and oleic acid (OA) that is stabilized with a plethora of nonionic methoxypoly(ethylene glycol) (mPEG)-lipids of different PEG chain length and variable lipid moiety. These nonionic stabilizers can modulate the internal architectures of these GMO/OA nano-self-assemblies.

Nanodispersion-mediated human complement activation was also examined. These safer stabilizer alternatives are attractive for preparing nano-self-assemblies that may serve as promising versatile injectable platforms for drug delivery, bio-imaging, and beyond. The research took advantage of small-angle X-ray scattering (SAXS), among others.

Publication

S. Yu Helvig, L. Woythe, S. Pham, G. Bor, H. Andersen, S. Moein Moghimi, A. Yaghmura, A Structurally Diverse Library of Glycerol Monooleate/Oleic Acid Non-Lamellar Liquid Crystalline Nanodispersions Stabilized with Nonionic Methoxypoly(ethylene glycol) (mPEG)-Lipids Showing Variable Complement Activation Properties. Journal of Colloid and Interface Science, Volume 582, Part B, 906-917 (2021). DOI: https://doi.org/10.1016/j.jcis.2020.08.085





HEALTH AND MEDICINE

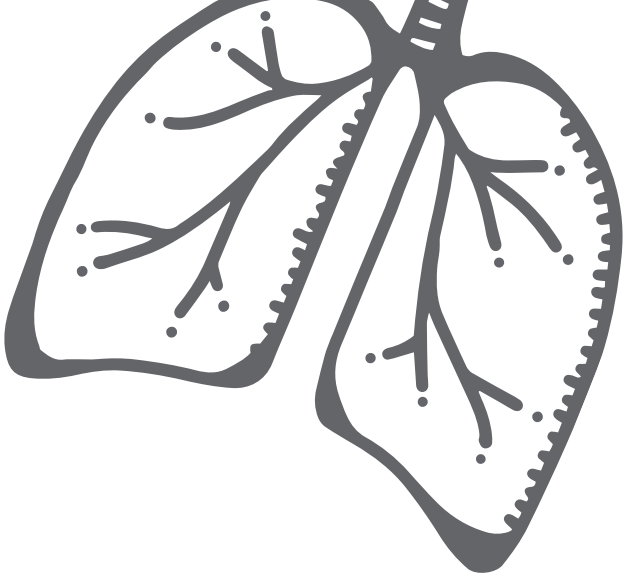
Zinc claim importance for skeletal bone formation

Human's long bone development is anchored on the gradual mineralization of a cartilage template. However, little is known on the smaller length scale of bone mineralization. Researchers from Lund University and Imperial College London characterized long bones' mineralization during embryonic development over a range of length scales (micrometre to nanometre) using the NanoMAX beamline. They focused on the murine humeri of mice, the equivalent of a long bone in a human's upper arm.

The study showed that Zn is essential for bone mineralization as it is a common co-factor of several enzymes which catalyze matrix mineralization. High Zn concentrations were identified in precise localization, specifically at the border of new and ongoing mineralization. NanoMAX provided the highest spatial resolution (nanometer) observation to confirm Ca and Zn's compositional/elemental distribution in the growth plate. These findings are essential in future studies to understand how different pathologies or pharmacological drugs may affect mineral deposition.

Publication

I. S. Barreto, S. Le Cann, S. Ahmed, V. Sotiriou, M. J. Turunen, U. Johansson, A. Rodriguez-Fernandez, T. A. Grünewald, M. Liebi, N. C. Nowlan, H. Isaksson, Multiscale Characterization of Embryonic Long Bone Mineralization in Mice. Adv. Sci. 7, 2002524 (2020), DOI: 10.1002/advs.202002524



HEALTH AND MEDICINE

Tackling antibiotic resistance through bacterial metabolisms

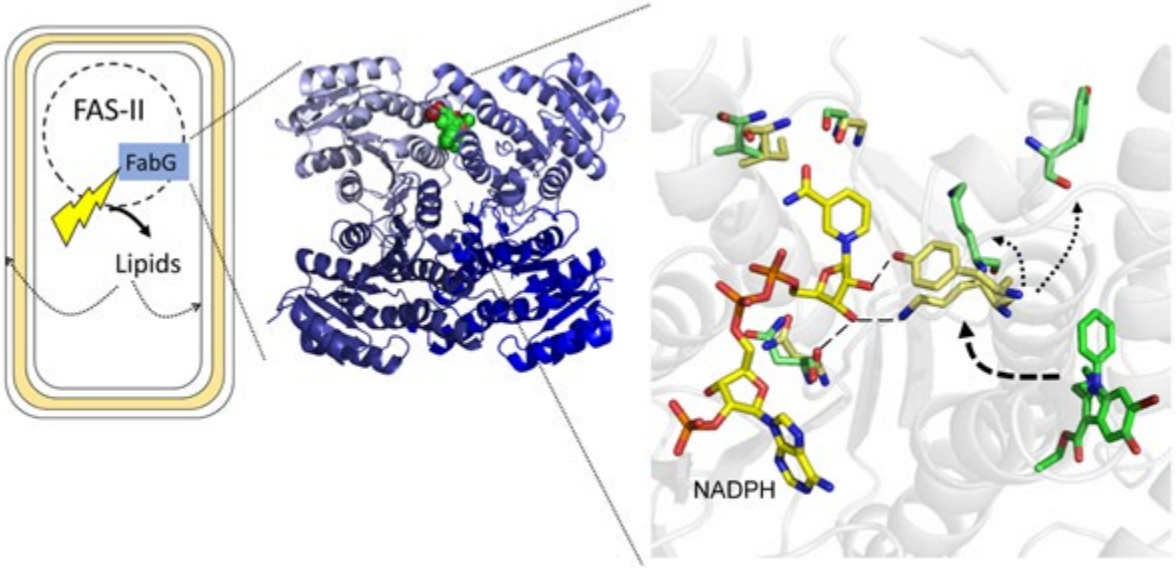
Global prevalence of antibiotic resistance to pathogenic bacteria is on the rise, most notable manifesting with serious infections in hospital environments or implants and medical devices. A study from the Karolinska Institute in Sweden characterized inhibitors for bacterial FabG proteins from S. typhimurium and A. baumannii, E. coli, M. tuberculosis, and others.

Researchers developed broad-spectrum inhibitors active on FabG enzymes for several pathogens. Binding of an inhibitor was found to distort the NADPH binding site in the A. baumannii enzyme. The structural change resulted in reduced NADPH affinity—identified as the mechanism of action that underlies the inhibitory effect.

The crystalline structure of the protein in complex with inhibitor was resolved with BioMAX beamline at MAX IV. In this age of emerging resistance, the work presents a novel candidate for antibiotic development targeting relevant metabolic pathways in bacterial pathogens.

Publication

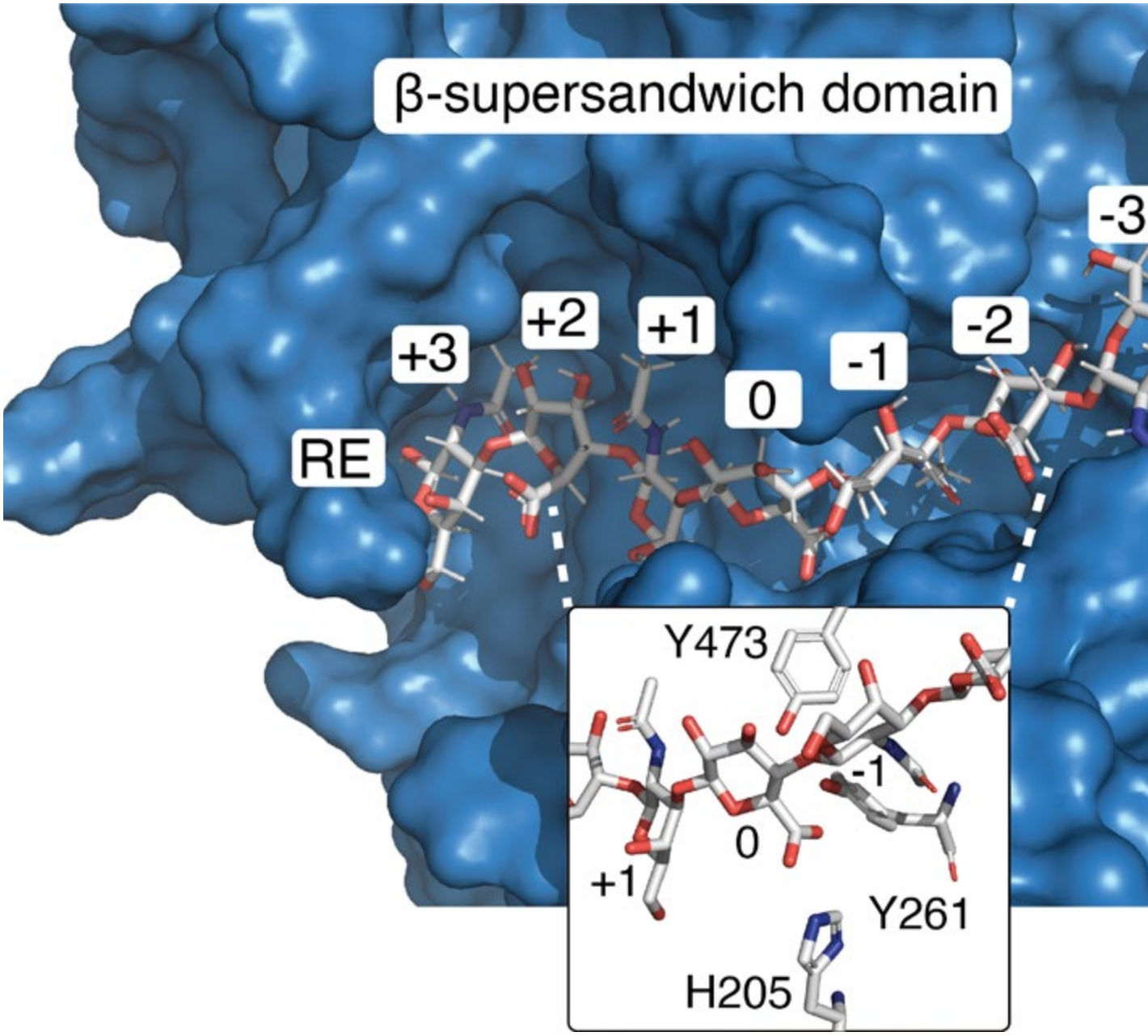
P. Vella, R. S. Rudraraju, T. Lundbäck, H. Axelsson, H. Almqvist, M. Vallin, G. Schneider, and R. Schnell, A FabG inhibitor targeting an allosteric binding site inhibits several orthologs from Gram-negative ESKAPE pathogens, Bioorganic & Medicinal Chemistry 30, 115898 (2021), DOI: 10.1016/j.bmc.2020.115898



Inhibitors idenified targeting FabG in the bacterial fatty acid biosynthesis pathway (FAS-II).

The top inhibitor binds at the subunit interface within the FabG tetramer.

The consequence of inhibitor binding at the subunit interface is the displacement of NADPH-coordinating residues.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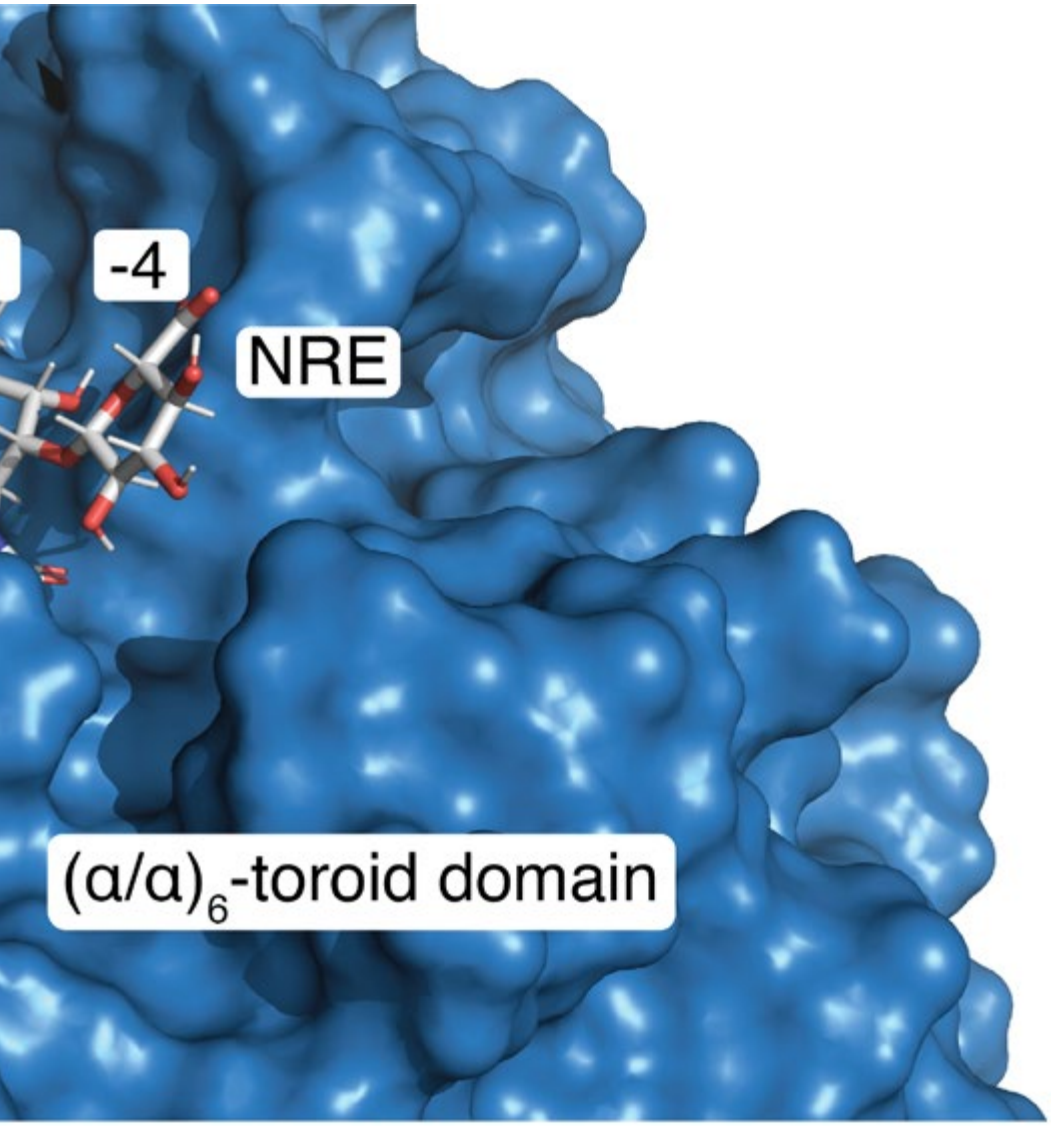


HEALTH AND MEDICINE

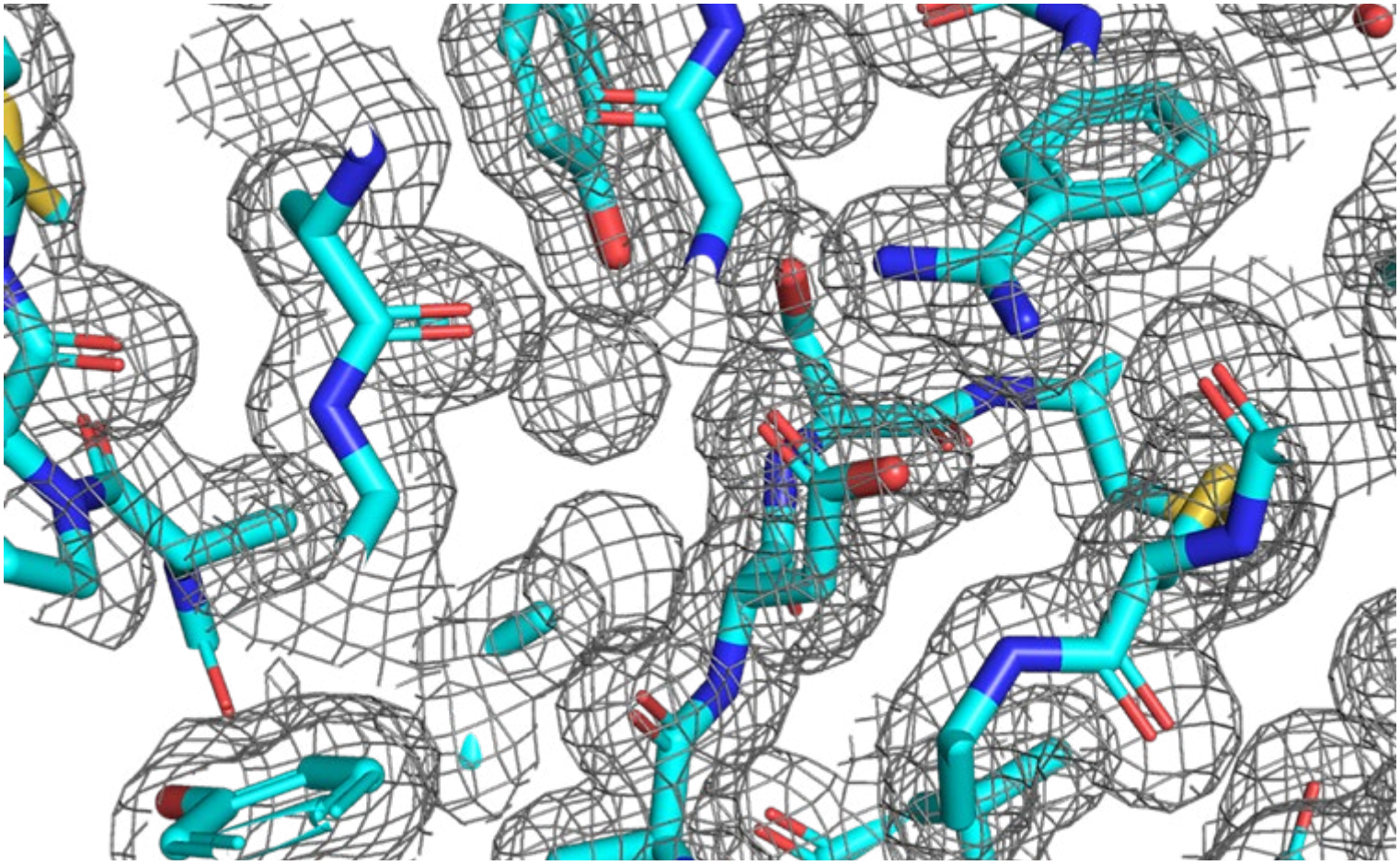
Enzyme structure of cancer-linked carbohydrate solved

The potential to slow progression of some cancers may be realised with greater structural and functional knowledge of a key enzyme involved in the biosynthesis of a complex carbohydrate, dermatan sulfate (DS), according to researchers at Lund University in Sweden. The DS carbohydrate/polysaccharide has a well-documented, but unresolved connection with metastasis and tumour growth.

A team at Matrix Biology lab has solved the crystalline structure of DS-epi1, a human enzyme which controls chemical reactions in cells related to DS biosynthesis, and gathered data on its mechanism. Crystalline samples were measured at BioMAX beamline at MAX IV. The findings offer a future possibility for molecule design and development of active-site inhibitors and new medications against various cancers and blood clotting diseases.

Publication

M. Hasan, H. Khakzad, L. Happonen, A. Sundin, J. Unge, U. Mueller, J. Malmström, G. Westergren-Thorsson, L. Malmström, U. Ellervik, A. Malmström, and Emil Tykesson, The structure of human dermatan sulfateepimerase 1 emphasizes the importance of C5-epimerization of glucuronic acid in higher organisms. Chem. Sci. **12**, 1869 (2021). DOI: 10.1039/d0sc05971d



ULTRAFAST SCIENCE

FemtoMAX suitable for time-resolved studies of protein dynamics

A team led by researchers from the University of Gothenburg have determined a novel use for the FemtoMAX beamline as an alternative to X-ray free-electron lasers in the study of time-resolved protein dynamics. The researchers used trypsin-crystals and recorded diffraction patterns at room temperature. After some adaption, the collected data could be analyzed using traditional X-ray crystallography software.

The researchers are interested in the role thermal fluctuations play in determining protein structure and function. In future experiments, the team also plan to trigger increased or squeezed fluctuations with ultrashort terahertz pulses. The dynamics of proteins are crucial to understanding protein function, such as how they communicate with one other in our cells or how the 3D complexity of the proteins, the cell, and the organism arises. Medical progress critically depends on how well we understand proteins.

Publication

M. Jensen, V. Ahlberg Gagnér, J. Cabello Sánchez, Å. U. J. Bengtsson, J. C. Ekström, T. Björg Ulfarsdóttir, M.-J. Garcia-Bonete, A. Jurgilaitis, D. Kroon, V.-T. Pham, S. Checcia, H. Coudert-Alteirac, Siawosch Schewa, M. Rössle, H. Rodilla, J. Stake, V. Zhaunerchyk, J. Larsson, and G. Katona, High-resolution macromolecular crystallography at the FemtoMAX beamline with time-over-threshold photon detection,
J. Synchrotron Rad. 28, 64 (2021), DOI: 10.1107/S1600577520014599

ULTRAFAST SCIENCE

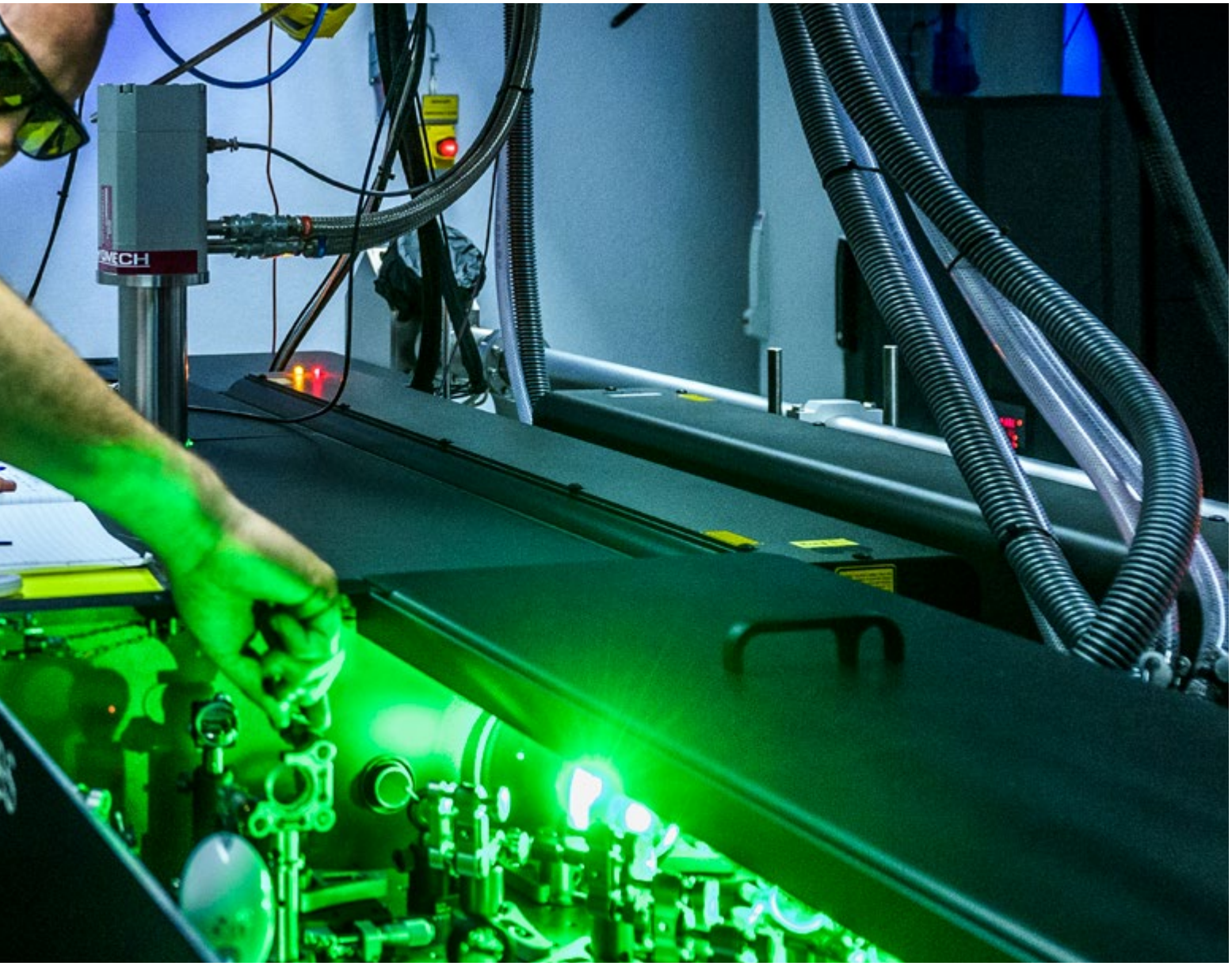
A luminescent material with sub-nanosecond time resolution

Many applications rely on luminescence detection with high resolution. Examples are time-of-flight positron emission tomography (TOF-PET) for medical imaging with a lower dose or calorimeters of future supercolliders in high-energy physics. Super-high time resolution is also important for monitoring radiation generated by free-electron lasers. The task is to find the right luminescent materials to realise the technology.

A collaboration of researchers from Lomonosov Moscow State University and Tartu University studied the luminescence kinetics of the material CeF3. They concluded the rise-on time on the scale of tens of picoseconds and the luminescence decay profile which predicts the structure and dimensions of excited regions. The CeF_3 crystal was investigated at MAX IV as well as DESY in Hamburg. A well-defined time structure of synchrotron radiation with picosecond pulses separated by hundreds of nanoseconds is ideal for this type of measurements.

Publication

I. Kamenskikh, E. Tishchenko M. Kirm , S. Omelkov, A. Belsky, and A. Vasil'ev, Decay Kinetics of CeF_3 under VUV and X-ray, Symmetry **12**, 914, DOI: 10.3390/sym12060914



ULTRAFAST SCIENCE

Atomic Vibrations Play Key Role in Material Phase Change

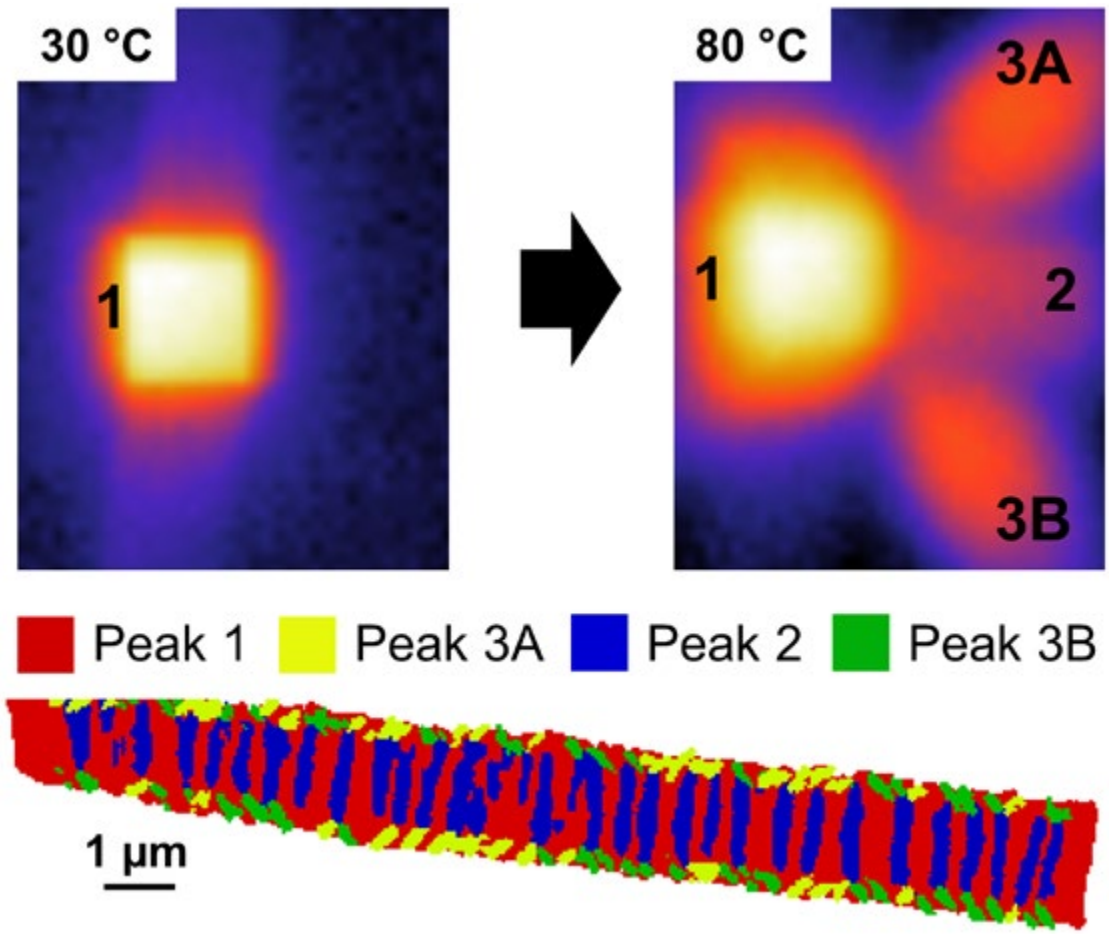
A research team from Lund University studied the non-thermal melting of indium antimonide (InSb) at the FemtoMAX beamline. The bonds in the material were broken with a femtosecond laser, and the process was probed with ultrafast X-ray pulses. The study revealed that the unbound atoms move with the velocity they had at the instant the bonds were broken.

Further, it showed that initial velocity is governed by atomic vibrations, which are temperature-dependent. The study provides evidence of the model of inertial motion. It verifies the need for new predictive models of atomic motion which take the initial velocities of atoms into account during phase change-laser interactions.

The findings are steps toward functional manipulation of the material structure during phase transitions. The result paves the way for improved and new innovative technologies such as the reading and writing of novel storage media, optical recording, and memory devices.

Publication

X. Wang, J. C. Ekström, Å. U. J. Bengtsson, A. Jarnac, A. Jurgilaitis, Van-Thai Pham, D. Kroon, H. Enquist, and J. Larsson, Role of Thermal Equilibrium Dynamics in Atomic Motion during Nonthermal Laser-Induced Melting, Phys. Rev. Lett. **124**, 105701 (2020), DOI: 10.1103/PhysRevLett.124.105701



ENERGY AND FUELS

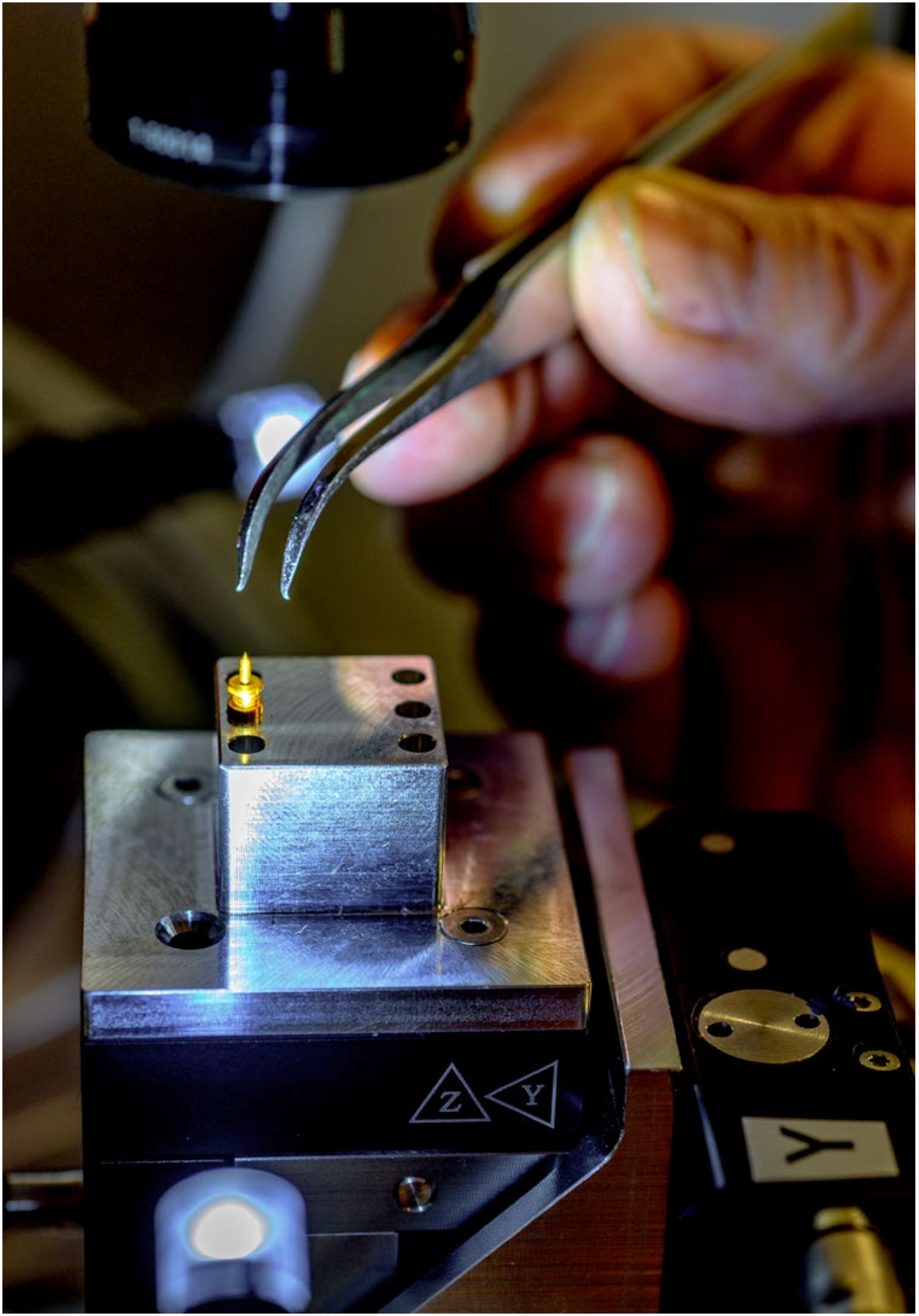
Imaging temperature-dependent ferroelasticity in perovskite nanowires

Metal halide perovskites (MHPs) could play an essential role in future solar cells and light-emitting devices. A group of international researchers produced and studied single-crystal nanowires of CsPbBr3, a highly stable MHP, to study the ferroelastic domains. Using scanning X-ray diffraction at the NanoMAX beamline, the researchers imaged the sample while gradually increasing the temperature. At 80 °C, a dramatic change in the crystalline order appeared with four new Braggs peaks, which the reciprocal space mapping concluded as a sign of ferroelasticity.

The domain pattern also became highly ordered at this temperature. The possibility to image individual ferroelastic domains using nano-focused X-rays, like NanoMAX, opens new possibilities to study and further develop other ferroelastic, ferroelectric, and multiferroic materials.

Publication

L. A. B. Marçal, E. Oksenberg, D. Dzhigaev, S. Hammarberg, A. Rothman, A. Björling, E. Unger, A. Mikkelsen, E. Joselevich, and J. Wallentin*, In Situ Imaging of Ferroelastic Domain Dynamics in CsPbBr3 Perovskite Nanowires by Nanofocused Scanning X-ray Diffraction, ACS Nano 14, 15973 (2020), DOI: 10.1021/acsnano.0c07426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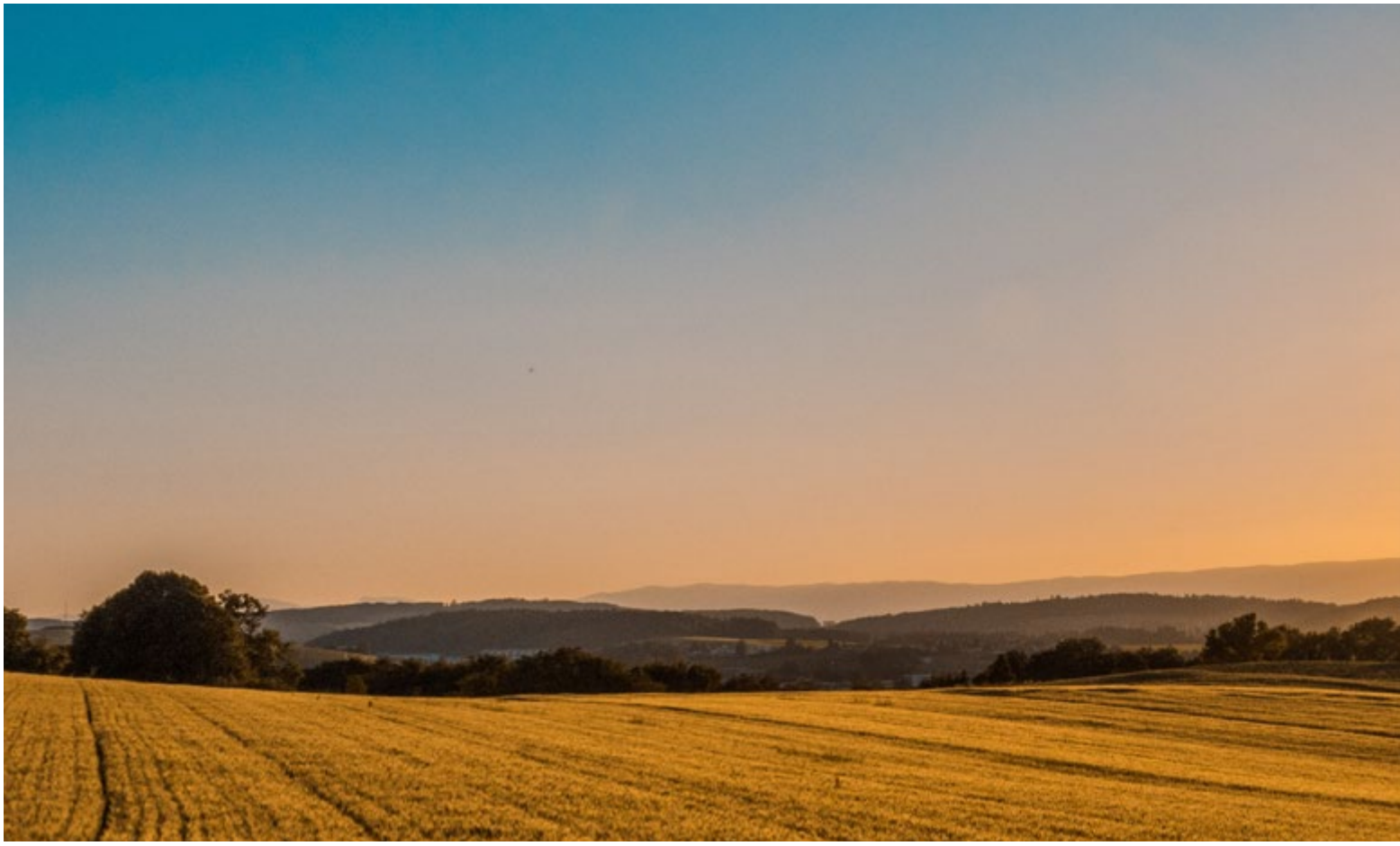


ENERGY AND FUELS

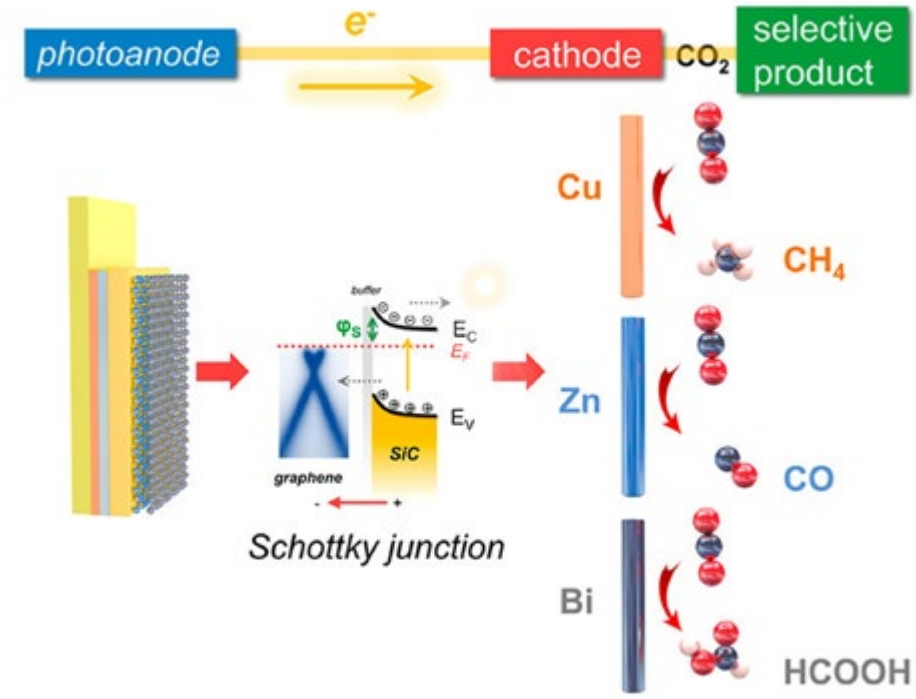
Chemical fuel produced with solar energy

A promising new method is under development to selectively convert carbon dioxide and water to various types of chemical fuel. Researchers at Linköping University in Sweden have combined the material graphene and the semiconductor cubic silicon carbide in a process which essentially mimics photosynthesis in plants. The Linköping group constructed a viable photoelectrode with adjustable Schottky junction.

With the application of solar energy, the graphene-semiconductor interface successfully produced a photoelectrochemical reaction to generate fuel. Low-energy electron microscopy (LEEM) and low-energy electron diffraction (LEED) characterizations of graphene were performed at MAXPEEM beamline at MAX IV. The production of fuels using solar energy offers an alternative to fossil fuels, and exploits graphene's unique material properties to build better sustainable, power applications.

Publication

H. Li, Y. Shi, H. Shang, W. Wang, J. Lu, A. A. Zakharov, L. Hultman, R. I. G. Uhrberg, M. Syväjärvi, R. Yakimova, L. Zhang, and J. Sun, Atomic-Scale Tuning of Graphene/Cubic SiC Schottky Junction for Stable Low-Bias Photoelectrochemical Solar-to-Fuel Conversion, ACS Nano **14**, 4905 (2020), DOI: 10.1021/acsnano.0c00986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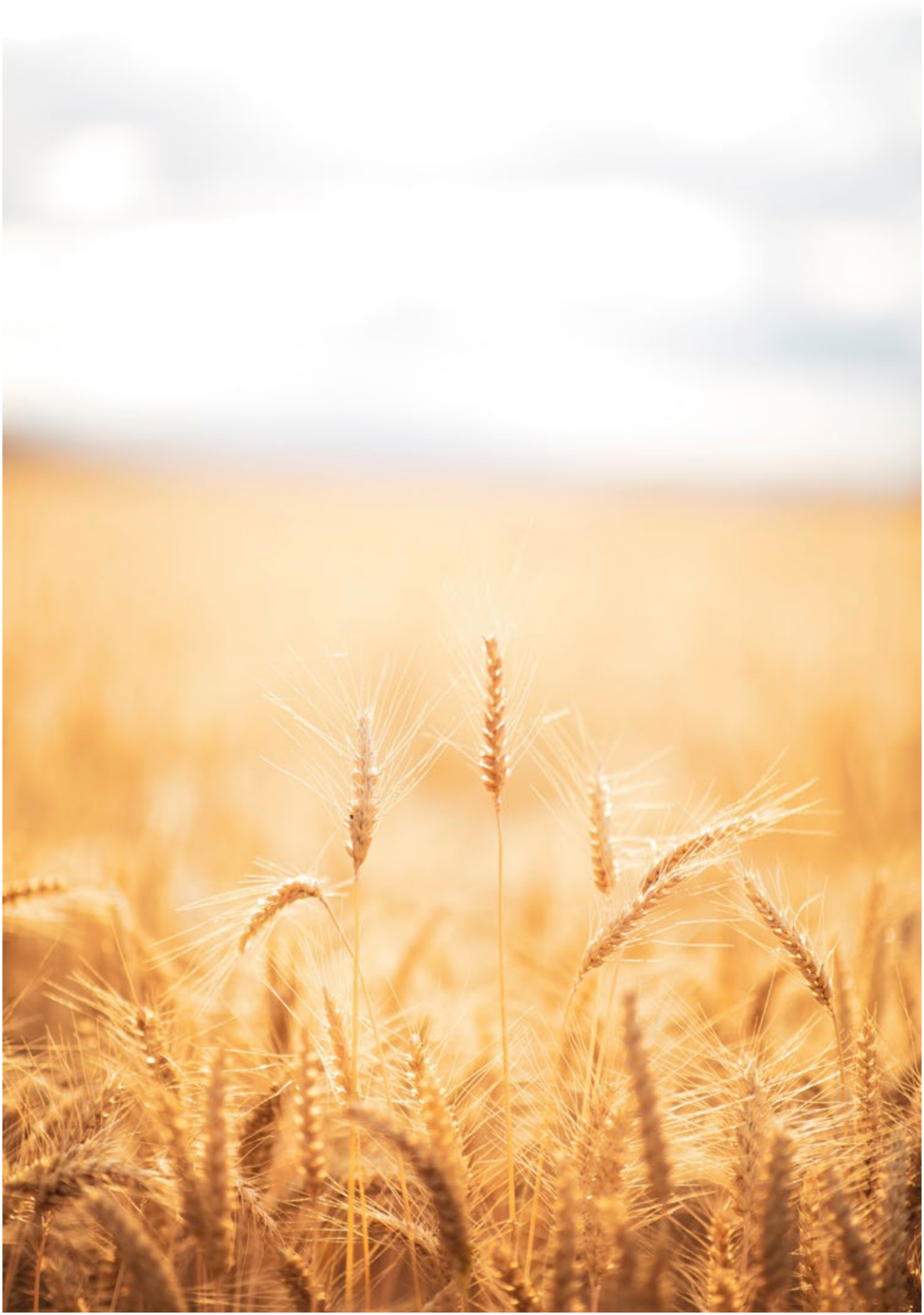
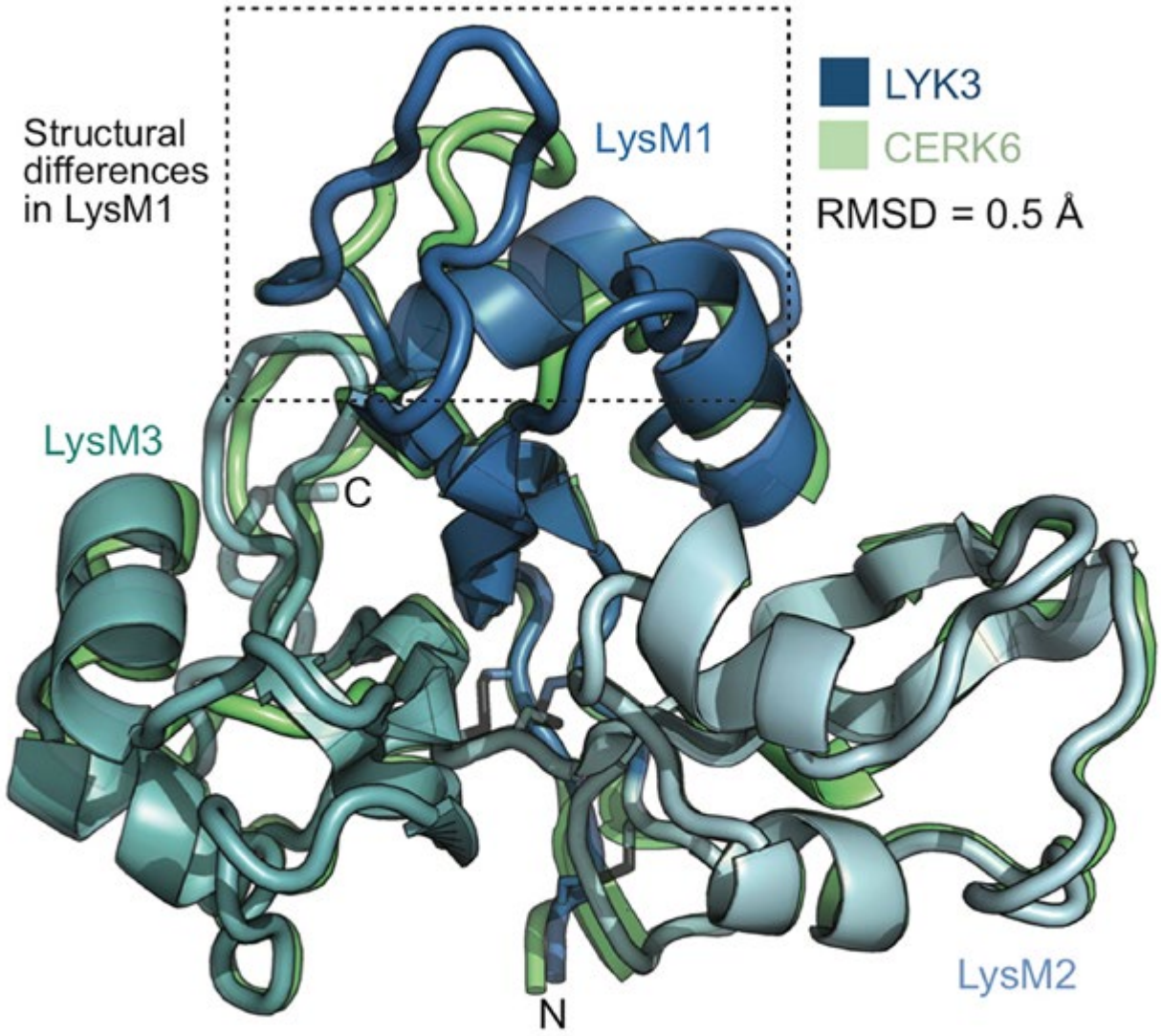
graphene
Schottky junction





STRUCTURAL BIOLOGY

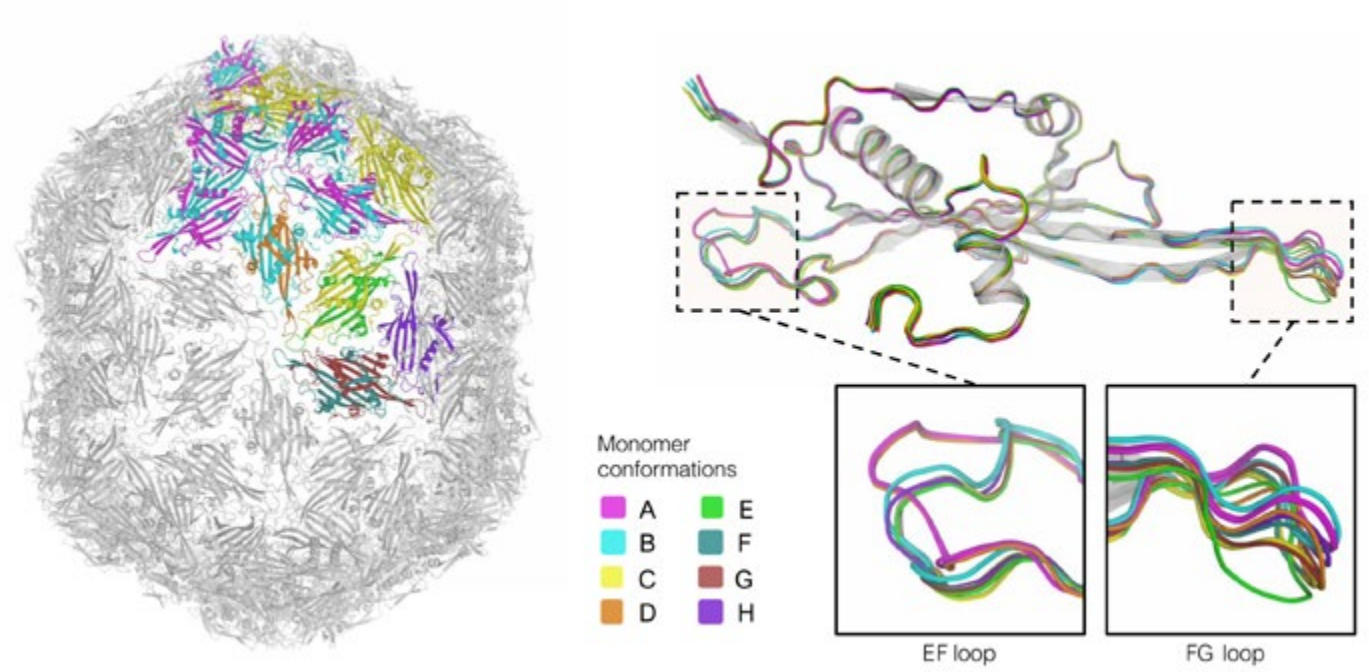
How plants distinguish harmful from beneficial bacteria

An international collaboration of researchers analysed how plants determine harmful from beneficial bacteria around them. Knowledge of the mechanism could enable engineering of new plant-microbe interactions for plant science applications. The study, led by Aarhus University in Denmark, examined the crystal structure of the symbiotic Nod factor (carbohydrates) receptor LYK3 at beamline I911-3 at MAX lab, and further, compared LYK3 to the chitin receptor CERK6 involved in immunity.

Results showed that LysM receptors establish signalling by using two specific motifs necessary for nitrogen-fixing symbiosis, and chitin-triggered immunity response against invaders. The researchers altered the LysM receptors and successfully converted a chitin immunity receptor to support symbolic signalling. The work demonstrates the capability to program receptors for different functions, an important step towards engineering nitrogen-fixing symbiosis into crops for more sustainable agriculture.

Publication

Z. Bozsoki, K. Gysel, S. B. Hansen, D. Lironi, C. Krönauer, F. Feng, N. de Jong, M. Vinther, M. Kamble, M. B. Thygesen, E. Engholm, C. Kofoed, S. Fort, J. T. Sullivan, C. W. Ronson, K. J. Jensen, M. Blaise, G. Oldroyd, J. Stougaard, K. R. Andersen, and S. Radutoiu, Ligand-recognizing motifs in plant LysM receptors are major determinants of specificity, Science 369, 663, DOI: 10.1126/science.abb3377



STRUCTURAL BIOLOGY

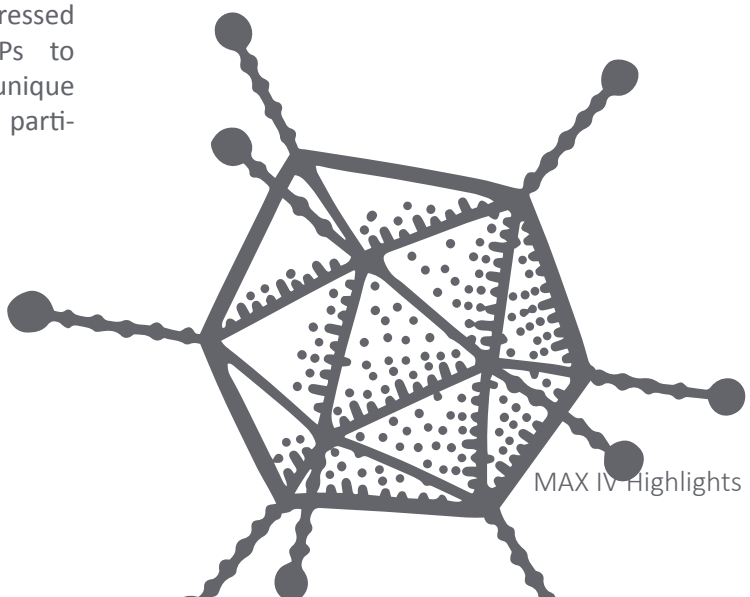
Tapping bacteriophages for vaccine development

A study from the Latvian Biomedical Research and Study Center has determined the three-dimensional structure of 22 previously uncharacterized single-stranded RNA (ssRNA) phage capsids with nine diverse coat proteins (CPs). Scientists looked at the bacteriophages—a group with simple, small genomes and high mutation rates—known to infect proteobacteria. Phages play a major role in our understanding of genome structure and function as well as viral evolution.

The Latvian group recombinantly expressed metagenome-derived ssRNA phage CPs to produce virus-like particles and found unique features in the phage coat protein fold, particle shape, and a previously undetected double-stranded RNA binding mode. X-ray diffraction data was taken at MAX-lab beamline I911-3 and MAX IV's BioMAX beamline. The results provide deeper insight of viral structural proteins and hold promise for the development of ssRNA-phage type vaccines in the future.

Publication

J. Rūmnieks, I. Liekniņa, G. Kalniņš, M. Šišovs, I. Akopjana, J. Bogans, and K. Tārs, Flexibility of the coat protein fold and variations in particle shapes. Sci. Adv. **6**, eabc0023 (2020). DOI: 10.1126/sciadv.abc0023



STRUCTURAL BIOLOGY

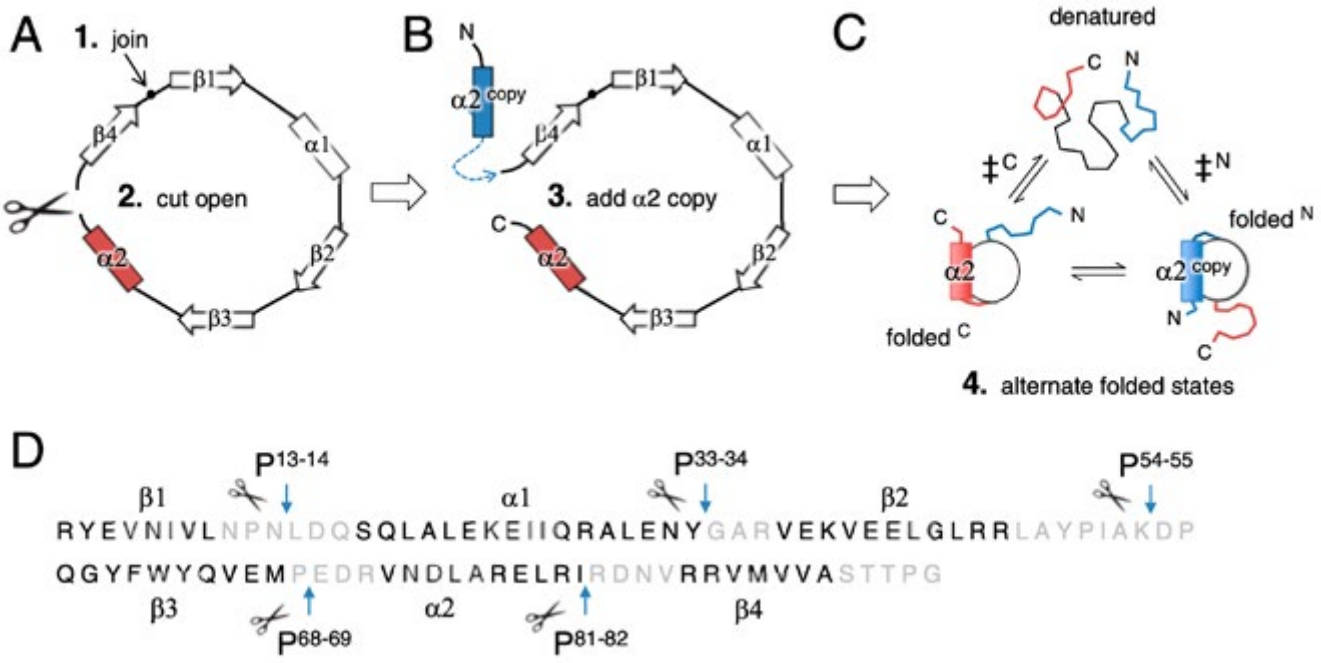
Designs reveal function, structure of folded proteins

A unique protein-design strategy developed by scientists at Stockholm University and Lund University reveals previously hidden behaviour and traits in folded proteins. Secondary elements of protein structure, composed of bundled beta strands and alpha helices, are notably difficult to study due to global folding cooperativity in the folding mechanism.

Through dynamic swapping of alpha and beta elements in folded ribosomal protein 6, the research group found beta strands remain anchored with local fluctuation until global folding occurs, whereas alpha helices can swap elements, hybridize in tertiary forms, and associate with other proteins by sliding onto nearby molecules. Crystallography data of the protein structure was collected at BioMAX beamline at MAX IV. The results further our knowledge of protein function, which may contribute to better models for protein design and tuning of protein structure.

Publication

H. Wang, D. T. Logan, J. Danielsson, and M. Oliveberg, Exposing the distinctive modular behavior of β-strands and α-helices in folded proteins, PNAS 117, 28775 (2020), DOI: 10.1073/pnas.1920455117



SCANNING PROBE MICROSCOPY

Essential step towards Wafter-Scale Graphene Nanoribbons

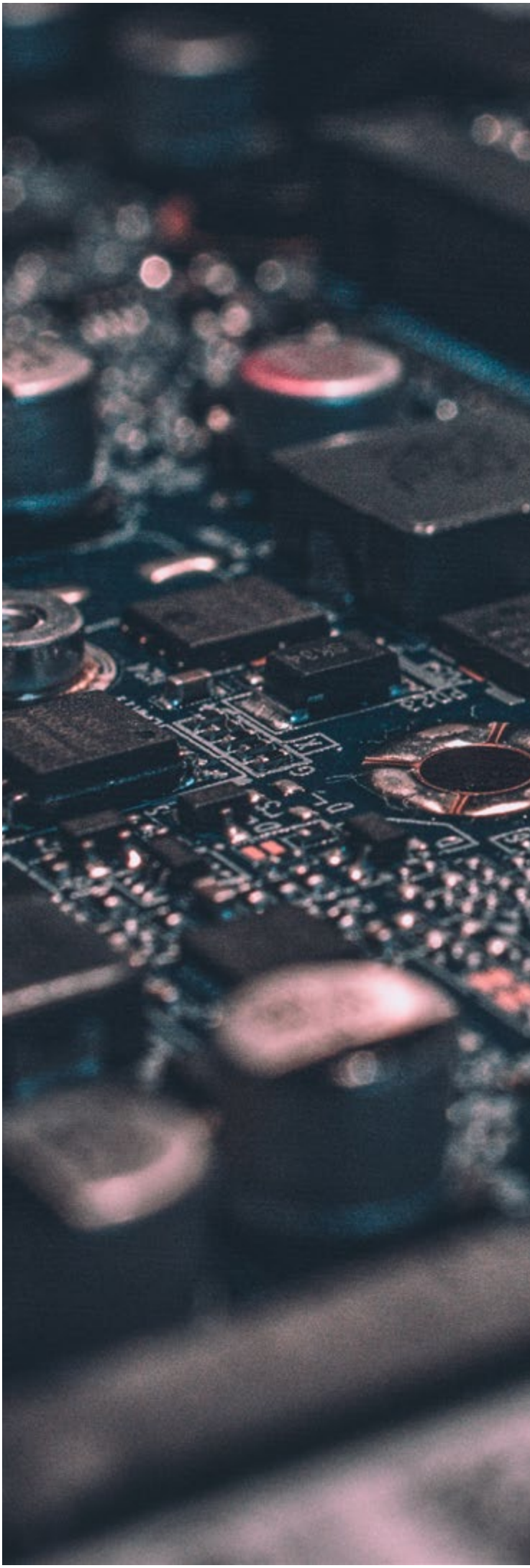
Low-dimensional systems are believed to be of great importance for the development of future electronics and spintronic devices. They also have unusual physical and chemical properties. A study led by Linköping University, and MAX IV, has taken an essential step towards wafer-scale fabrication of atomically precise graphene devices. The study is a part of a bigger European project called Tailspin.

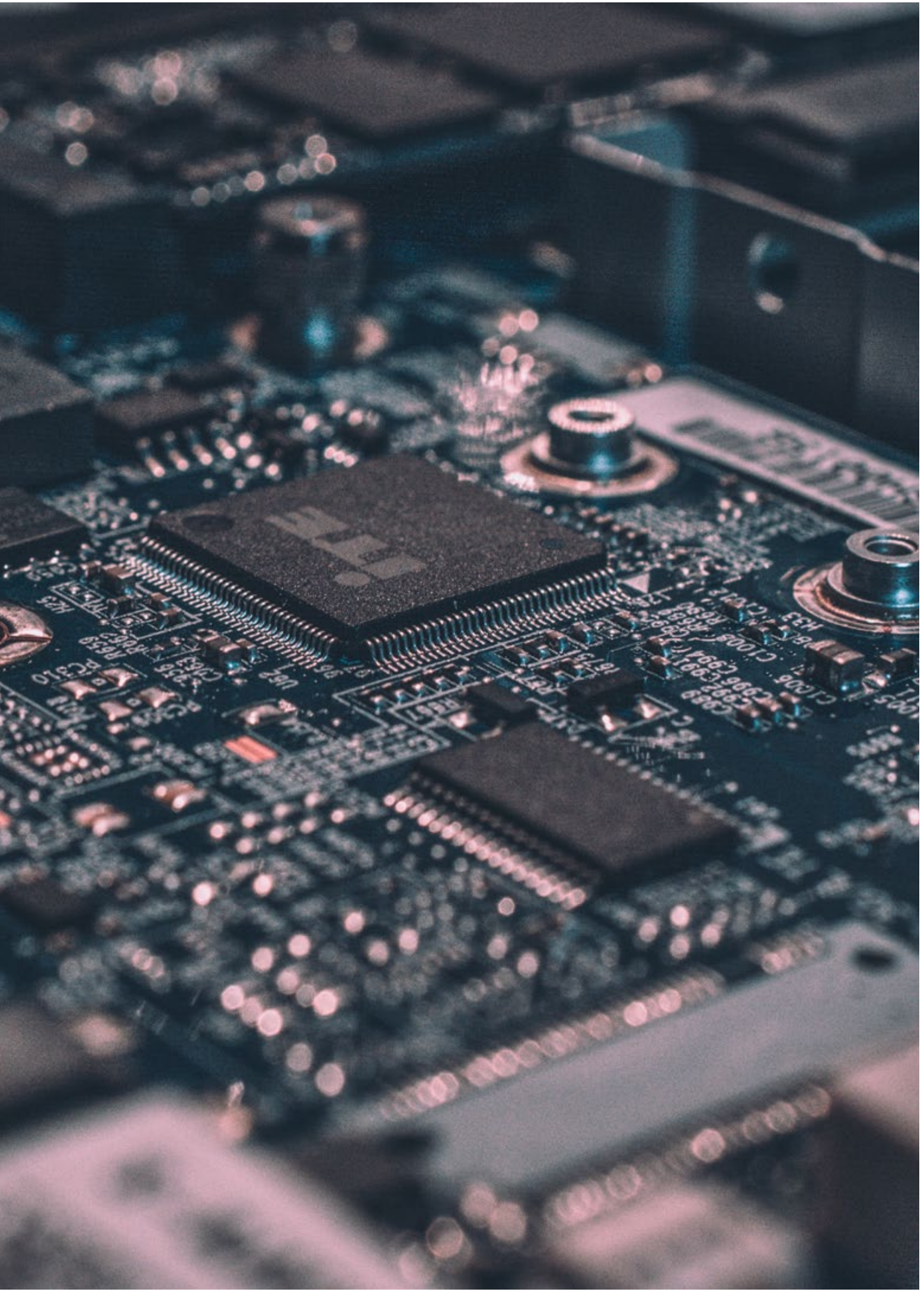
It is possible to grow edge-specific graphene nanoribbons showing unique transport properties. The ribbons with the zig-zag edges show ballistic transport of charge carriers, while the ribbons with the armchair edges demonstrate a gap opening in the electronic spectrum. To get these properties, the graphene nanoribbons must be structurally almost perfect and maintain the same atomic arrangement of their edges over micrometre lengths.

The research team used Scanning Probe Microscopy and Low-Energy Electron Microscopy (LEEM) at the MAXPEEM beamline to confirm the cornerstone assumption on the specific structure of the Graphene Nano Ribbon edges.

Publication

Y. Shi, A. A. Zakharov, I. G. Ivanov, N. A. Vinogradov, G. R. Yazdi, M. Syvajarvi, R. Yakimova, J. Sun, A patterning-free approach for growth of free-standing graphene nanoribbons using step-bunched facets of off-oriented 4H-SiC(0001) epilayers, J. Phys. D: Appl. Phys. 53, 115102 DOI: 10.1088/1361-6463/ab6149





FragMAX – a new facility for early-stage drug discovery

FragMAX is a new user facility for crystallographic fragment screening at MAX IV Laboratory. The facility is accessible to Swedish and international scientists from academia and industry. It provides simple workflows for large-scale crystal preparation, data collection and analysis. Users with different levels of experience are enabled to routinely find starting points for drug development.

The FragMAX facility provides an easily accessible and generic platform for scientists wanting to find starting points for chemical probe or drug development. Crystallographic fragment screening at the beamline BioMAX builds on the experience of MAX IV Laboratory for providing access to advanced infrastructures to a diverse user community. The facility offers efficient workflows to expert groups from industry who want to diversify their screening cascade. It also enables academic researchers to kickstart early-stage drug discovery projects that are otherwise restricted to well-equipped industrial groups.

The contribution of academic groups to drug development is of utmost importance, because the process is often hampered by insufficient target validation, i.e. there is often too little evidence available that modulation of a particular protein target with small molecule drugs will lead to the desired therapeutic effect in the clinic. Companies, therefore, rely on academia for pre-clinical

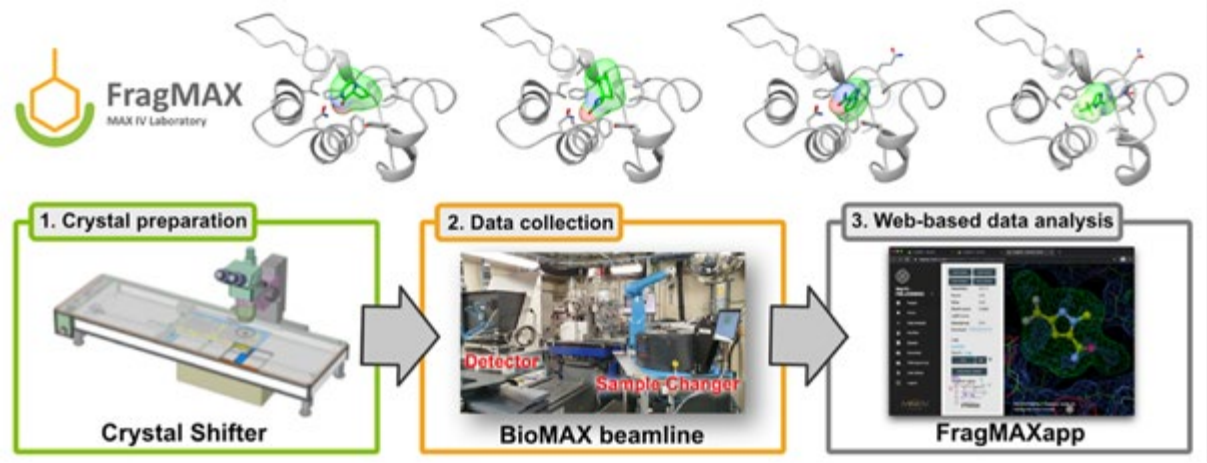


Figure 1. (top) Exemplary hits (green) from a crystallographic fragment screening campaign at FragMAX. (bottom) Overview of the different components of the FragMAX facility. (1) a semi-automatic crystal mounting stage enables preparation of hundreds of samples per day; (2) the high-intensity X-ray beam at BioMAX combined with a fast detector and a quick sample-changing robot facilitate high-throughput data collection; (3) FragMAXapp provides a convenient and intuitive data processing and analysis web application.

validation of novel targets and FragMAX provides them with a platform for the exploration of new ideas.

Fragment-based lead discovery
Fragment-based lead discovery (FBLD) is by now an established drug development strategy that has so far delivered 5 novel drugs and there are currently more than 40 FBLD-derived drug candidates in clinical trials. Starting points for lead development are found by screening of hundreds of fragment molecules. FBLD has several conceptual advantages over lead discovery by high-throughput screening, notably, the small library sizes and reduced logistics required for initial screening make it an attractive method for academic groups, who otherwise cannot access expensive high-throughput methods.
A platform with three components FragMAX provides a publicly available platform for crystallographic fragment screening at BioMAX, the first operational beamline for macromolecular crystallography at MAX IV. Crystal-based screening by X-ray diffraction is one of the most sensitive and information-rich methods because it provides a detailed 3D image of the protein-fragment interaction that directly informs the drug design process.

FragMAX consists of three main components:

- A crystal preparation facility at LP3 diffraction data collection at BioMAX
- An intuitive web-based tool for large-scale data processing (FragMAXapp)
- Access and libraries

Access to the facility is free of charge for academic users. Industrial groups can get access through

the MAX IV Industrial Relations Team. FragMAX provides free access to four distinct fragment libraries which encompass more than 1200 chemicals, without any restrictions on intellectual property.

Crystal preparation is supported by a semi-automated mounting stage (Crystal Shifter) that enables preparation of hundreds of samples per screening campaign for subsequent data collection at BioMAX. Finally, an intuitive web application for large-scale data analysis (FragMAXapp) enables users to process, visualize and analyze their data while being in their home labs. The platform is user-friendly and supports the needs of novices and experts alike.

Funding
Development of the FragMAX facility is funded by the Swedish Research Council (Grant 2018-06454). Additional funding from VINNOVA enabled development of sensitive data handling within FragMAXapp (Grant 2019-02567). The project receives support by iNEXT-Discovery, project number 871037, funded by the Horizon 2020 program of the European Commission.

Publications

Lima, G. M. A. et al. FragMAX: the fragment-screening platform at the MAX IV Laboratory. Acta Cryst D 76, 771–777 (2020).

Lima, G. M. A. et al. FragMAXapp: crystallographic fragment-screening data-analysis and project-management system. Acta Cryst D 77, (2021).

MAX IV Accelerators

Overview

Despite the restrictions imposed by the COVID-19 pandemic, the MAXIV accelerators continued to provide high performance and reliability throughout 2020 and all operational goals for the year have been achieved or surpassed. Operating under pandemic restrictions has proven to be a challenge in several respects. Significant effort has been devoted to making accelerator operations, troubleshooting and studies as much as possible remotely.

The operation involved administrative measures such as limiting the number of people in the control rooms, as well as implementing efficient mechanisms for remote operation of accelerator subsystems. At the same time, a number of new significant accelerator and engineering developments have been successfully implemented and the Accelerator Division groups continued providing the needed support, adapting to working from home whenever possible. We also note that all of the effort put into developing tools and procedures to cope with COVID-19 have provided us with new capabilities, which will be very useful even after the pandemic is over, allowing, for example, on-call staff to fix problems remotely and faster.

Early in 2020, the top-up injection period in the 3 GeV ring was changed from 30 to 10 minutes with a corresponding reduction of the beam intensity variations in-between top-ups. The beneficial effects could be confirmed by observations made with X-ray beam position monitors at various beamlines. At the same time, further trimming of the Multipole Injection Kicker (MIK) developed in collaboration with synchrotron SOLEIL and installed in 2019 allowed reaching sub-micrometre perturbation level at injections into the 3 GeV ring. Also in the 3 GeV ring, further analysis of the non-linear optics based on a newly developed method (NOECO) led to significant improvement of the momentum acceptance with a positive effect on the beam lifetime.

Finally, a fast orbit feedback was brought into routine operation in autumn, which brings the orbit perturbations produced by insertion device gap movements down to below 10% of the electron beam sizes.

In the 1.5 GeV ring, much attention was devoted to the compensation of perturbations produced by insertion devices (IDs) with the first two phases of a four-phase project aimed at removing any restrictions to operation of the IDs being completed. In addition, the operation of transverse-resonance island buckets (TRIBs) has been further explored with dedicated experiments performed in collaboration with the beamlines.

The increase of the repetition rate of the linear accelerator from 2 Hz to 10 Hz both for delivery to the short pulse facility (which provides short electron bunches to the FemtoMAX beamline) as well as for injection into the storage rings was demonstrated in autumn and has been the standard mode of operation since November 2020.

Finally, the bulk of the technical work related to the conceptual design report for a soft X-Ray Free electron laser (SXL) driven by the MAX IV 3 GeV LINAC (Figure 1) was completed and writing up of the final version was ongoing in the end of 2020 with the final editing foreseen for early 2021.

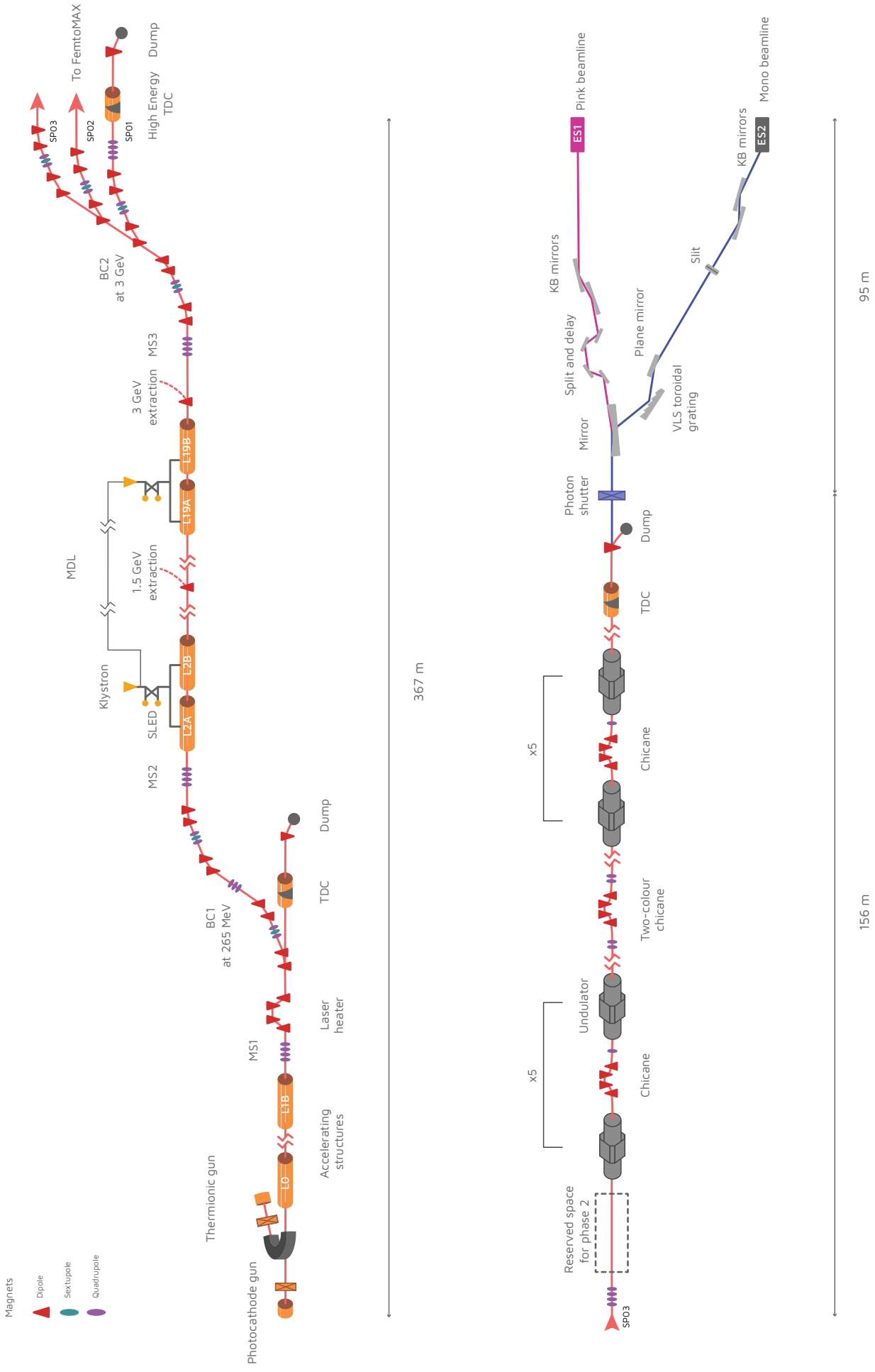
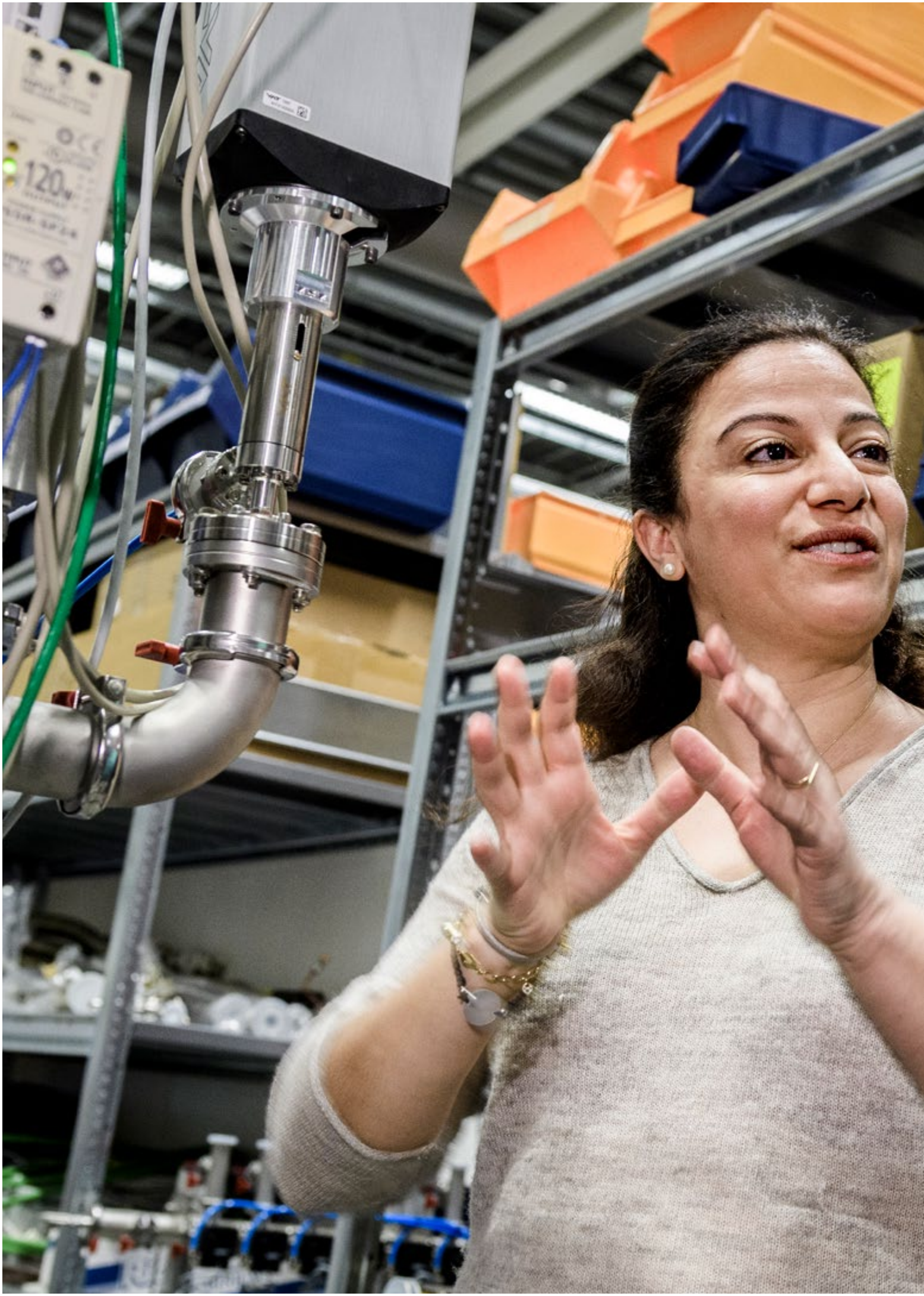
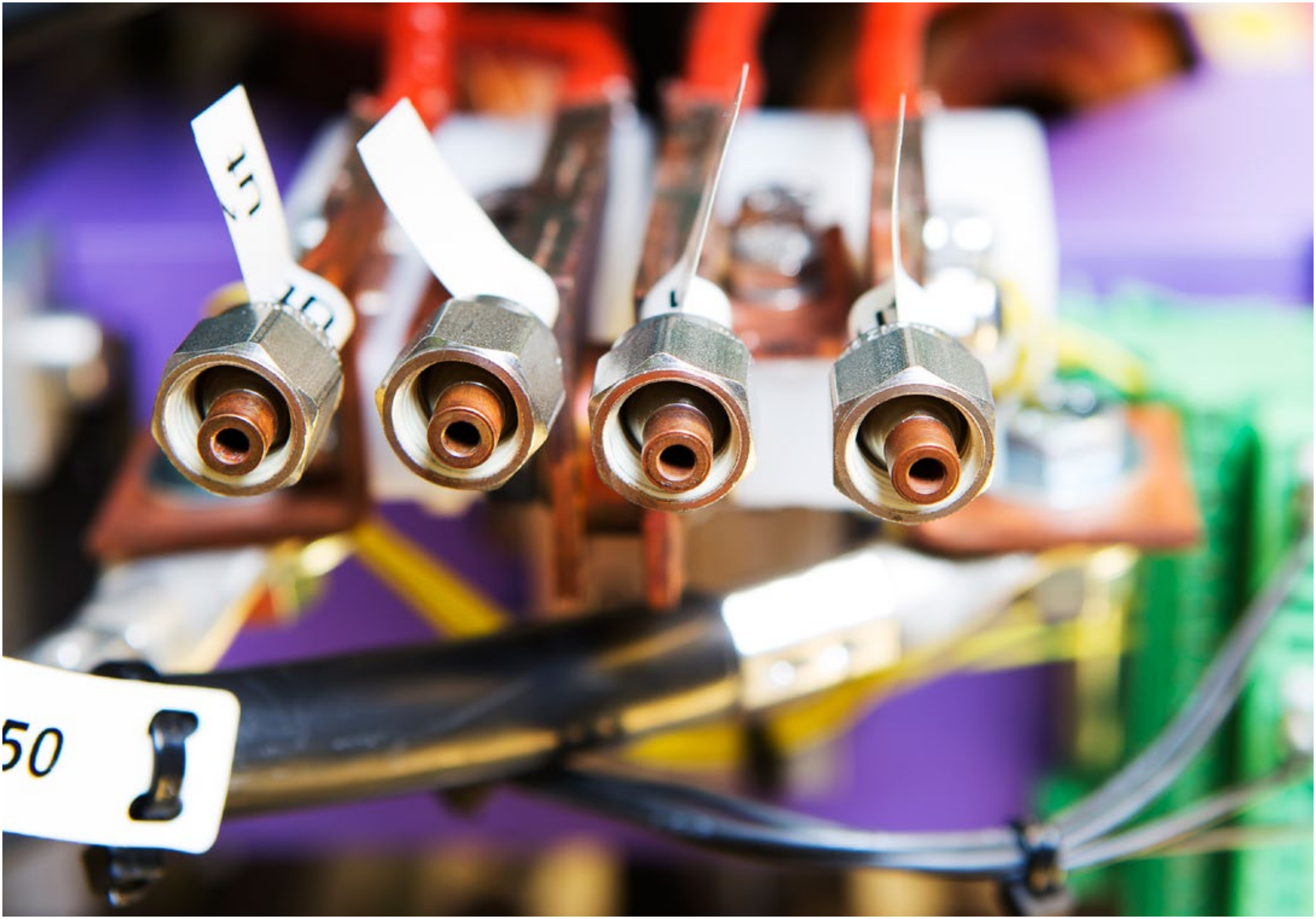


Figure 1: SXL Layout. top - existing system with improvements. Right – new systems

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Accelerator operations

The year 2020 will be remembered for the huge challenges posed by the COVID19 pandemic. In particular was the need to continue to run the three MAXIV accelerators while almost all of the technical experts were required to work at home for long periods. Despite this, it is with significant pride that we can report that the MAXIV accelerators continued to operate according to plan throughout the year. For the Accelerator Operations group, the most direct impact of the pandemic was the strong restrictions placed on access to the control room, which required only one accelerator operator to be in on-site while another one worked from home.

To compensate for this, significant efforts went into the installation and development of digital tools. Following the Zoomification that the rest of the working world has experienced, several video- and text-based communications applications were installed in the accelerator control room, thereby allowing face-to-face real-time conversations between operators and various technical experts.

In addition, remote access software was installed on several workstations to allow control of certain accelerator functionality from off-site. These tools significantly eased the work of operating and developing the MAXIV accelerators.

The accelerator availability statistics in 2020 are shown in Table 1. We note that the availability goals of >97% for the rings and >95% for the SPF were achieved. The availability can be thought of as a combination of the "Mean Time to Repair" (MTTR) and the "Mean Time Before Failure" (MTBF), where the MTTR is the average time it takes to respond to and fix a downtime, and the MTBF is the average time for which the accelerator operates as it should. While the MTTR for our accelerators is very good, we struggled with a poor MTBF.

To tackle this, we started in 2020 a so-called "MTBF Taskforce", to investigate and implement ways to improve these statistics. The statistics clearly showed that a large fraction of the downtimes on both rings were triggered by minor vacuum events in the beamlines.

It was clear that these were dominated by a class of events that posed no risk to the operation of the beamline or the accelerator, and so did not require such a strong reaction. A project has been initiated to reconfigure the Machine Protection System of the beamlines to respond differently to these events and is expected to be completed for all storage ring beamlines by 2022.

Table 1: Accelerator Operation Statistics in 2020

Accelerator	Delivery (h)	Downtime (h)	Availability (%)	MTTR (h)	MTBF (h)
R1	5104	98.0	98.1	1.1	56.1
R3	4872	126.8	97.4	1.0	39.9
SPF	4584	198.6	95.7	0.7	15.6

3 GeV ring

Transparent injection

The Multipole Injection Kicker (MIK), developed in collaboration with SOLEIL Synchrotron and installed in summer 2019, was fine-tuned and further characterized in spring 2020[1]. After optimization of the transverse position of the electron beam inside the kicker, the stored beam size perturbations at top-ups were brought down to sub-micron levels (Figure 1), arguably a world record. For comparison, the horizontal/vertical beam size at the centre of the long straights are on the order of 50/3 µm.

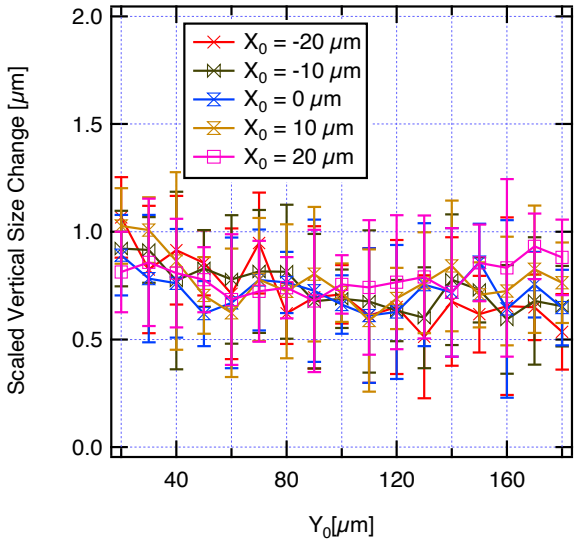

Figure 1: Vertical beam size perturbation as a function of vertical position of the store beam as it crosses the MIK.

Fast Orbit Feedback

Over the past year, the combined Slow Orbit Feedback and Fast Orbit Feedback system in the 3 GeV ring has been extended from a local system around the NanoMAX ID straight to cover all ID straights in the 3 GeV ring. The global system went into operation in October and has proven itself capable of eliminating orbit transients due to changing ID gaps (Figure 2), which were the main source of disturbances.

The overall closed orbit noise stability, as measured by the integrated power spectral density, was already within tolerances. Nonetheless, some improvement in the horizontal plane could be seen. Further planned improvements expected for the coming year include the increase of the closed-loop bandwidth in the vertical plane, currently limited to 40 Hz.

Non-linear electron beam optics characterization

In order to calibrate the higher-order optical elements in the 3 GeV ring, specifically the chromatic sextupoles, a new method called NOECO (Non-linear optics from off energy closed orbits) has been developed at MAX IV. As the widely used LOCO (Linear optics from Closed Orbits) method of calibrating the linear optics, it also relies on measuring orbit responses due to corrector magnet excitations and fitting an optics model to produce the same response. The difference lies in performing these measurements at different beam energies, which allows probing of the chromatic sextupoles. The method was further refined in 2020 and is now in regular use at MAX IV and is considered also at other fourth-generation light source facilities[2].

RF system

Over the past year, efforts to improve the Mean Time To Recover (MTTR) included implementing a measurement system for the relative phases

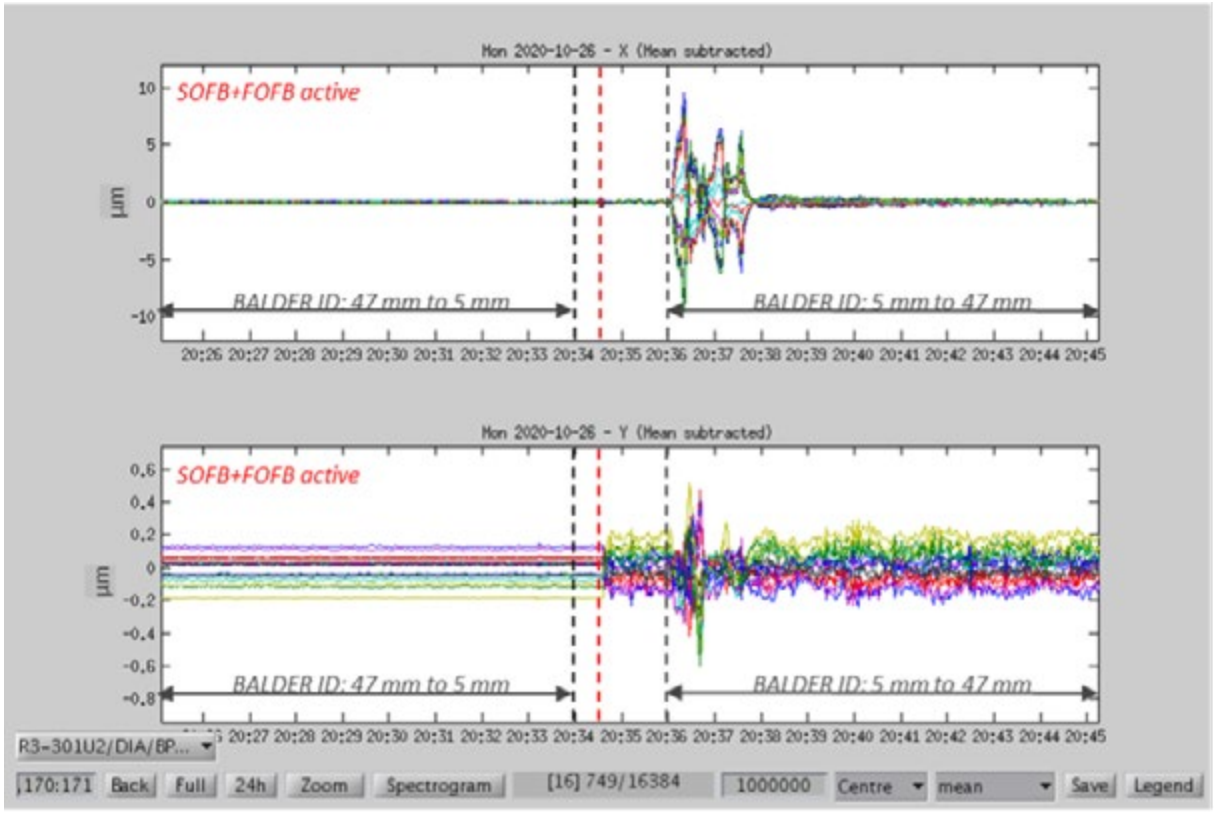

Figure 2: Orbit distortion at BPMs flanking the beamline ID straight sections while closing and opening the BALDER in-vacuum wiggler. The transients are largely eliminated with the combined SOFB and FOFB system active.


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between the R3 cavities, which has significantly sped up the re-phasing process. The LLRF system saw significant performance improvements for the TANGO devices with greatly improved update rates (15-20x faster) and improved control of the harmonic cavities. A flat-potential feedforward for automatic adjustment of main and harmonic cavity field levels to the energy-loss per turn (ID gaps) and current level was implemented in TANGO. Finally, a large body of work was done on characterizing and tuning the six 100 MHz RF cavities and three passive 300 MHz harmonic cavities. This included temperature tuning to allow running with all six main cavities powered, thus increasing the rf power margin available to cope with present and future insertion devices. It also meant refining and testing a Higher Order Mode (HOM) model for all the installed cavities, and a significant amount of work to stabilize the beam using the harmonic cavities[3].

Vacuum system

The past year has brought further confirmation of the successful implementation of the innovative vacuum system design of the 3 GeV storage ring, where almost 100 % of the vacuum chambers are coated with NEG (Non-Evaporable Getter). The experience gathered over five years of operation provides invaluable information to

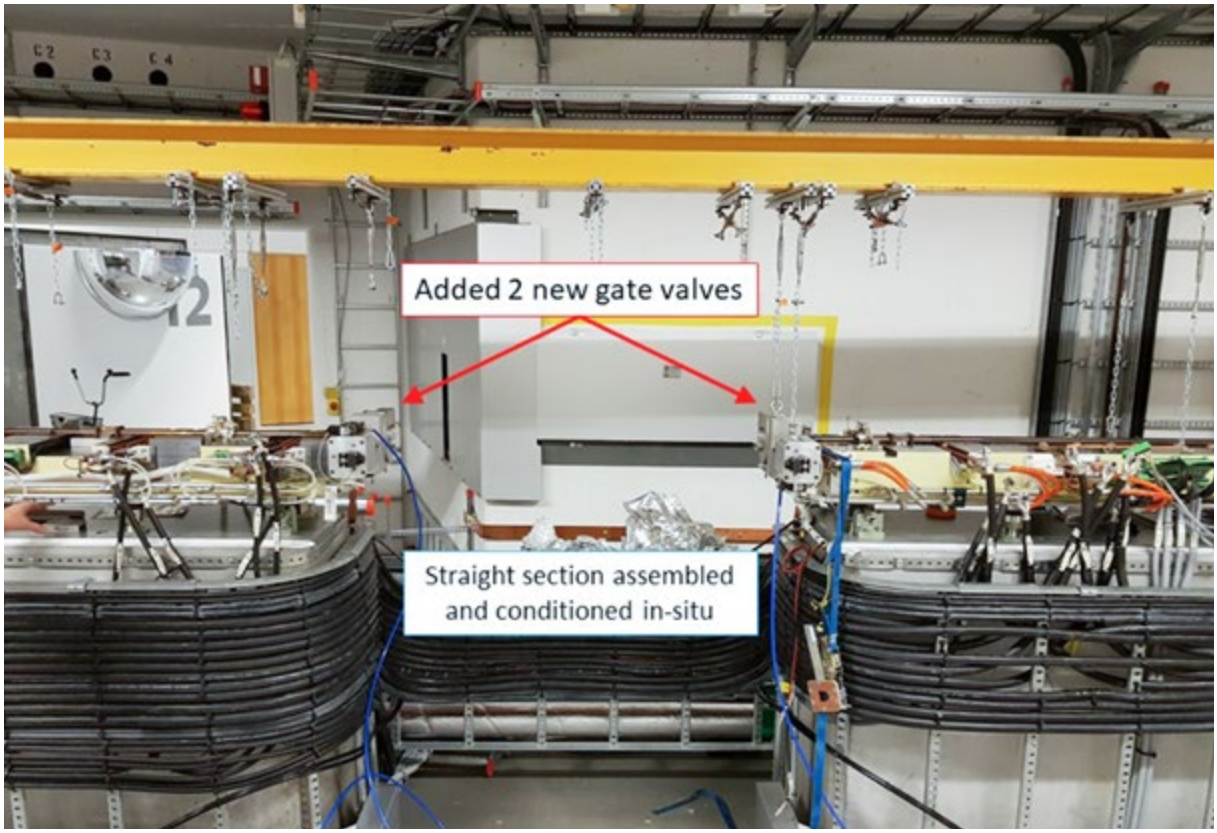


Figure 3: Two gate valves are added to a short straight in achromat 12.

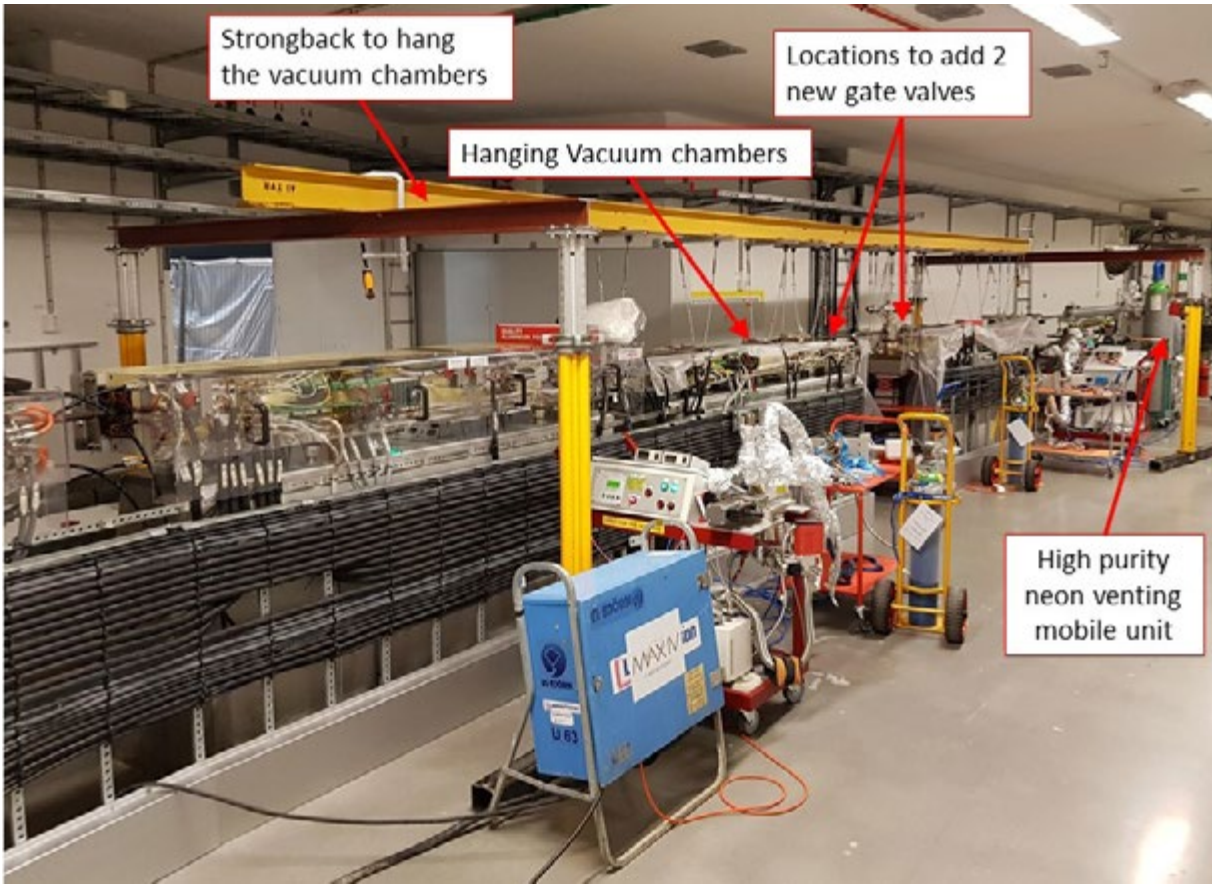


Figure 4: Preparing for a neon-venting intervention in achromat 12.

the synchrotron community currently actively engaged in the design of new fourth generation storage ring based light sources.

During the 2020 summer shutdown, two vacuum gate valves were installed in preparation for the future installation of a 5th harmonic rf cavity (Figure 3 and 4). For this, the neon-venting procedure that was first used by MAX IV at a synchrotron light source a couple of years ago, was employed: one 22-m-long achromat was vented with high purity neon gas, which allowed fast recovery of excellent vacuum lifetime in just a few days, without the need for re-activation of the NEG coating.

[1] p. Alexandre, R. Ben el Fekih, A. Letrésor, J. da Silva Castro, F. Bouvet, J. Breunlin, Å. Andersson, P. Fernandes Tavares, Transparent top-up injection into a fourth-generation storage ring, NIM A **986**, 164739 (2021), DOI: 10.1016/j.nima.2020.164739

[2] D. K. Olsson, Å. Andersson, M. Sjöström, Nonlinear optics from off-energy closed orbits, PRAB 23, 102803 (2020), DOI: 10.1103/PhysRevAccelBeams.23.102803

[3] F. J. Cullinan, Å. Andersson, P. F. Tavares, Harmonic-cavity stabilization of longitudinal coupled-bunch instabilities with a non-uniform fill, PRAB 23, 074402 (2020), DOI: 10.1103/PhysRevAccelBeams.23.074402

1.5 GeV ring

Work on compensating the perturbations produced by the five insertion devices in the 1.5 GeV ring continued in 2020. This work is necessary to prevent a reduction in beam lifetime and/or injection efficiency at certain gaps and phase settings of the elliptically polarizing undulators.

The focus of the work in 2020 was on providing compensation for the linear (focussing) effects of the IDs, which comprise the first two steps of a four-phase project. These first two phases compensate the (up-right) linear optics perturbations with local ring magnets surrounding the ID. Phase three covers the skew linear compensation needed for inclined and “universal” polarisations and phase four covers the non-linear compensation needed for the two strongest elliptically polarising undulators (EPUs) BLOCH and FinEst. The latter is most likely not possible to accomplish with ring magnets, and therefore so-called current strips will be implemented on the ID-chambers in question. Phase three is planned for 2021 whereas phase 4 is planned for 2022.

The operation of a transverse resonant island bucket operation was further developed during the year. This mode of operation aims to allow for simultaneous delivery of single bunch and multi-bunch for the users. Additionally, it allows for a relatively fast switching between the two modes. Focus in 2020 has partly been to theoretically explore the particle dynamics close to the third order resonance in the ring, partly to find the practical solutions for a delivery mode that is as robust as the present multi-bunch delivery mode. A third focus has been to work together with the beam lines for finding the best ring settings for an optimum separation of the beam orbits at the specific beamlines.

The choice has been to separate the orbits in the horizontal direction at the third order resonance, resulting in three separated orbits together with the ordinary core orbit. For an efficient use of the extraordinary orbits, where the single bunch is placed, the beamlines need to verify that they are able to block all but one of the extraordinary orbits. Depending on the beamline photon optics, particular settings of first and succeeding mirrors were chosen. Additionally, the orbits appear differently in different straight sections where the IDs are situated, which of course also entails individual beamline solutions. Nevertheless, such solutions were found, and we expect the work during 2021 to be concentrated on the robustness of this mode of operation.

Linear Accelerator

A major milestone for the linear accelerator in 2020 was the increase of the repetition rate of the electron pulses from 2 to 10 Hz, a development that has included both technical and operational efforts as well as radiation safety risk analysis and a new permit from the Swedish Radiation Safety Authority (SSM). 10 Hz is the designed repetition rate for injection into the storage rings.

In SPF mode, the accelerating phase in the two first linac sections was re-tuned to fit with the so-called “Magic Angle” where the particular bunch compression scheme at MAX IV reaches a very high stability with respect to HV and phase fluctuations from the RF units. This, together with improved phase feedback, allows the arrival time for the electron bunches to SPF to reach a very high stability. After the above-mentioned improvements an energy stability consistent with an arrival time jitter of 10 fs RMS was measured.

Precision realignment of the entire LINAC

The MAX IV accelerators have hundreds of components that need to be precisely positioned not only relative to one another but also with respect to the global coordinate system of the facility. This requires high-precision alignment of sensitive components through a multiple-stage process including survey, data analysis, establishment of a reference network, fiducialisation and realignment. During the past two years the linear accelerator was realigned [1] and the developed methods serve as a guide for large-scale realignment problems that involve surveying, outlier analysis, fiducialisation, boundary conditions, solution/optimization of reference networks, and physical realignment of the components.

[1] B. Afzali-Far, A. Andersson, K. Zhou, M. Malmgren, Data analysis, spatial metrology network, and precision realignment of the entire MAX IV linear accelerator, Nucl. Instrum. Methods Phys. Res., Sect. A **1003**, 165267 (2021), DOI: 10.1016/j.nima.2021.165267.

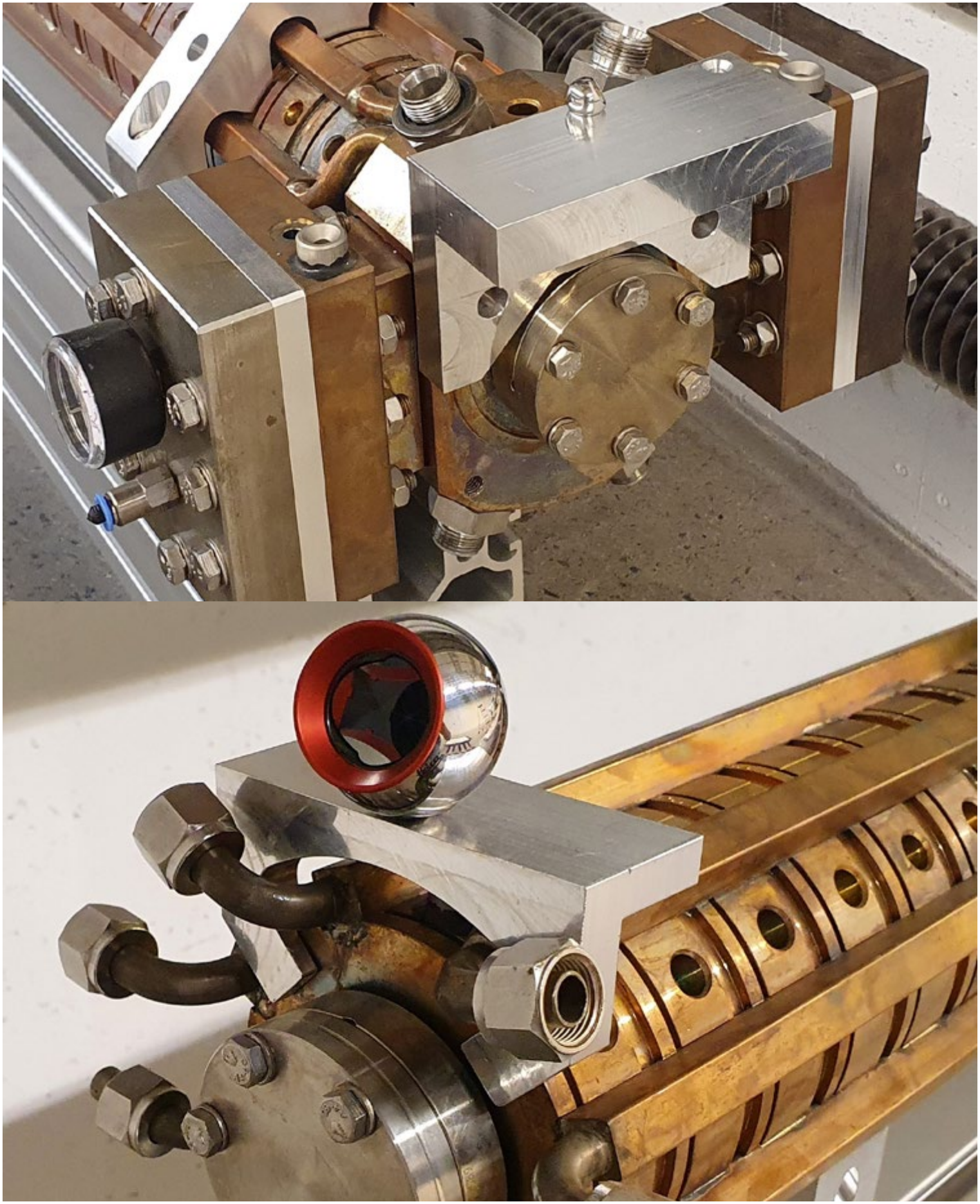
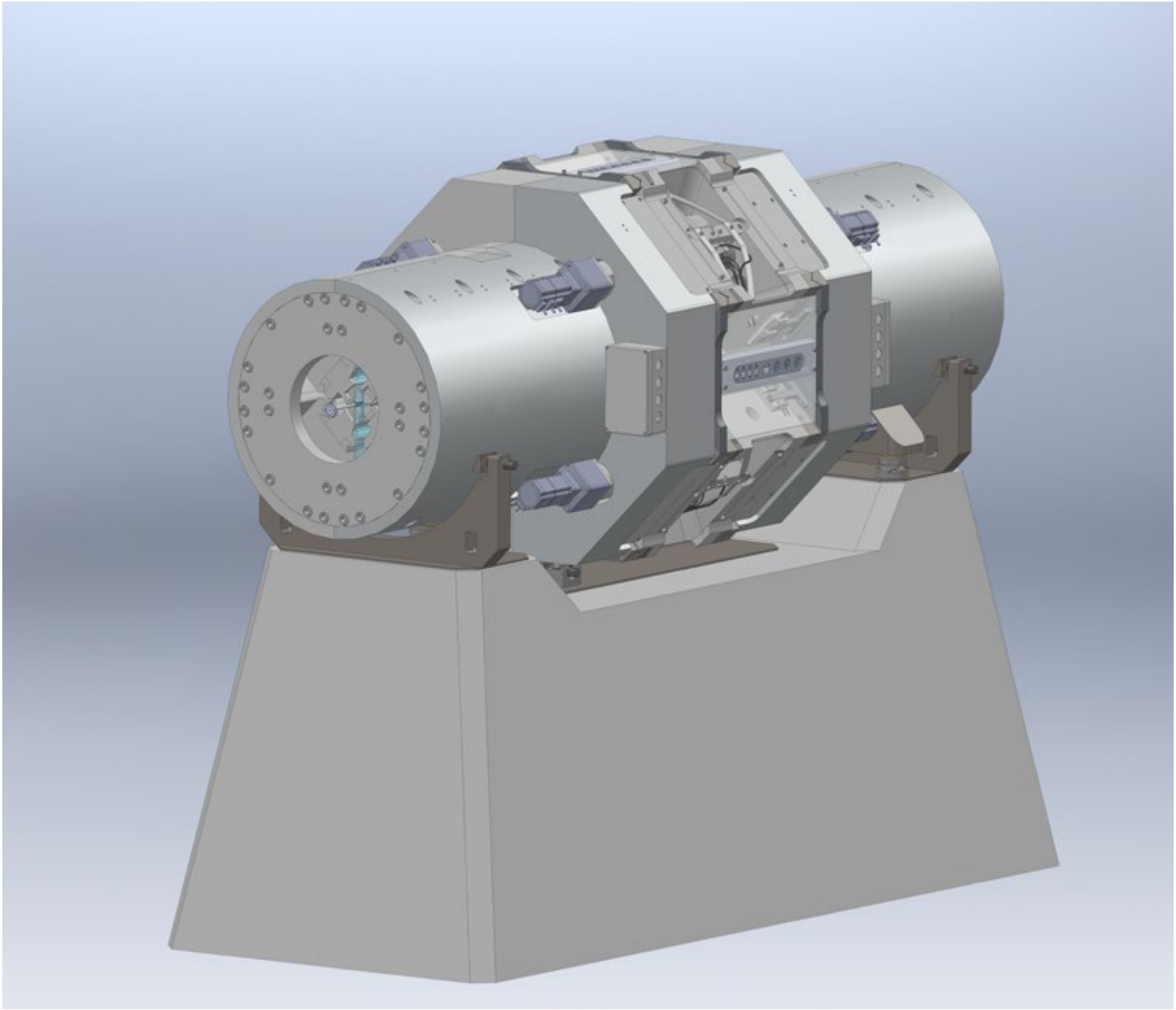


Figure 1: The adaptors designed for measuring the accelerating structure: upstream (top),downstream (bottom).

Apple X Insertion Device

The proposed SXL will be driven by the 3 GeV electron beam from the MAX IV linear accelerator to produce photons in the 1-5 nm wavelength range. The undulator line of SXL is based on the use of a compact APPLE X structure newly designed at MAX IV. A full-scale prototype of the compact APPLE X is currently under construction.

The period length is 40 mm and the magnet blocks material is based on Samarium Cobalt.The detailed design is in the final stages for a compact APPLE X undulator with a round aperture of diameter of 8 mm. The design will be cost-effective solution compared to the existing APPLE II and provides full polarization control with constant effective K-value as a function of phase, i.e., polarization state.



Engineering Developments

B.O.R.I.S. – the bluelining robot
Bluelining is a technique of transferring a three-dimensional computer model into real space providing marks for equipment installation on the floor. In order to avoid the time-consuming manual bluelining process, MAX IV is developing, in collaboration with the Faculty of Engineering at Lund University (LTH), a high-precision self-positioning robot that simplifies the work by automatically driving to the location specified by a computer and marking that position with a dot and lines.

The robot development involves students from a number of courses and activities at LTH such as Applied Mechatronics, Applied Robotics, Control and learning and Engineering Training. A presentation of the project at the EU Robotics week was done in 2020 and a Master thesis entitled "Mobile Floor-Marking Robot, utilizing Feedback from Laser Tracker" by Lisa Klinghav was completed. The system aims at an accuracy better than 0.1 mm and a repeatability better than 0.02 mm.

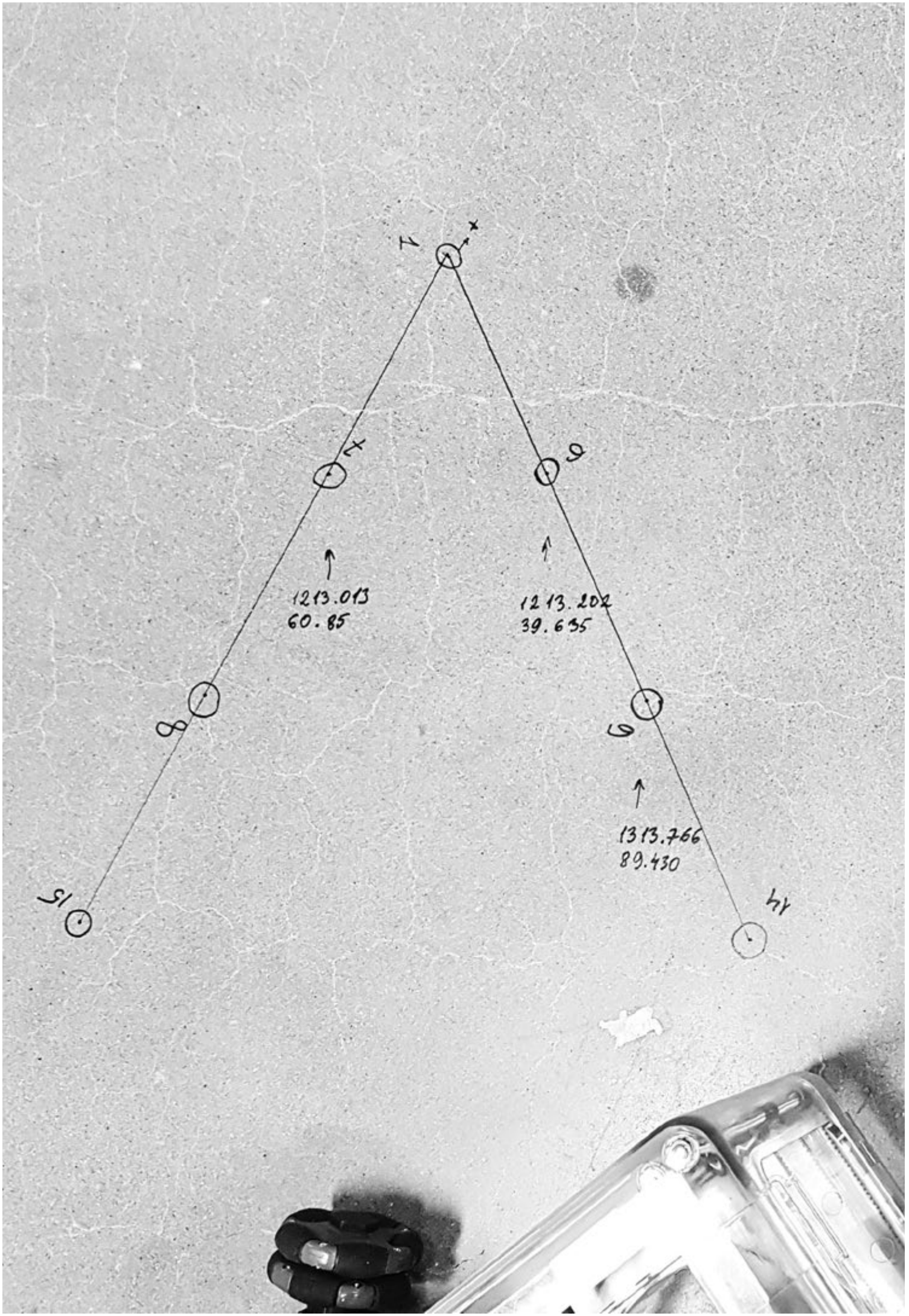
Mechanical stability, vibrations
Having vibration levels under control is critical when it comes to the stable operation of the accelerator and the beamlines. The foundation of the MAX IV building, whose vibration sensitivity was considered from the very beginning of the building design, has proven to be effective in minimizing the adverse effects of traffic on the E22 motorway. Recently most attention has been directed towards handling internal sources of vibration and supporting the design of future beamlines.

Long term vibration monitoring is a useful tool to find already existing internal vibration sources based on their unique vibration signatures. The information obtained this way can be used to identify, locate and eventually isolate vibration generating equipment which may disturb sensitive experimental instrument. Today we monitor a few isolated locations but plans are under way to extend this system to overview the entire facility.

To minimize vibrations of sensitive equipment it is crucial to understand the dynamic behaviour of the entire supporting structure. At MAX IV, experimental techniques are used to characterize existing structures and to extract important dynamic parameters from prototypes. Providing designers with the results of these tests can improve the vibration properties of future beamlines.

Precision Mechanics Design
Precision mechanics design is a central ingredient in various ongoing synchrotron radiation instrumentation developments at MAX IV. Figure 10 (left) shows the the flight tube for the ForMAX beamline which has a diameter of 1 m and a total length of 8.8 m with removable end section for easy access.

The internal rails of the flight tube are decoupled from the vacuum vessel which give better stability. Figure 10 (right) shows the sample table for the MicroMAX beamline, which has a total of six motorized legs and the ability to handle 200 kg payload with micrometre level motion accuracy.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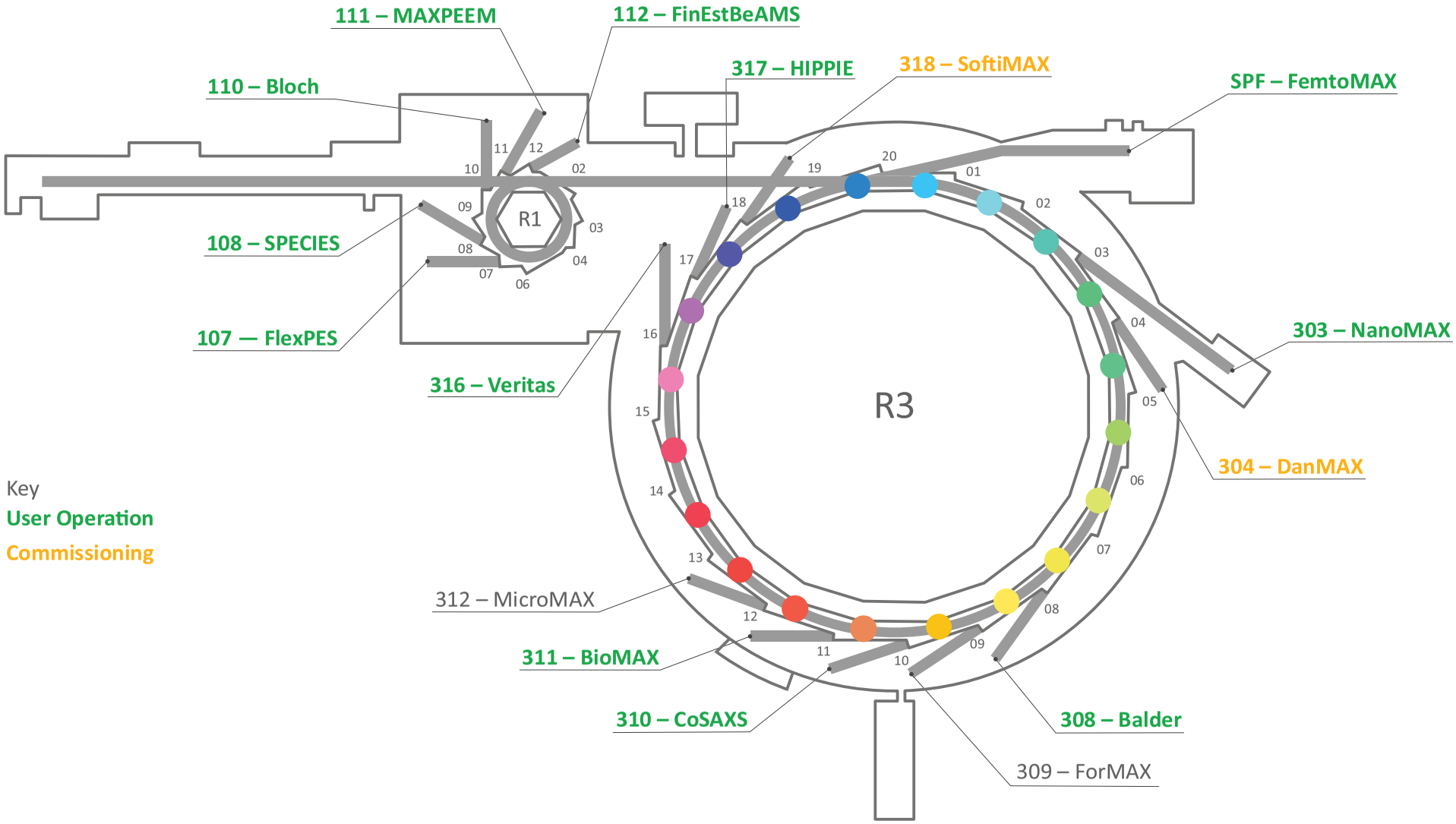
Facts and Figures


111 – MAXPEEM
112 – FinEstBeAMS
110 – Bloch
317 – HIPPIE
318 – SoftiMAX
SPF – FemtoMAX
R1
108 – SPECIES
107 — FlexPES
316 – Veritas
R3
303 – NanoMAX
304 – DanMAX
Key
User Operation
Commissioning
312 – MicroMAX
311 – BioMAX
310 – CoSAXS
308 – Balder
309 – ForMAX

Beamline	Accelerator	Methods
Balder	3 GeV	Hard X-ray absorption and emission spectroscopy (XAS, XES) w and X-ray diffraction (XRD) with emphasis on in-situ and time resolved studies
BioMAX	3 GeV	Macromolecular crystallography with a high degree of automation and remote user access
Bloch	1.5 GeV	Angle resolved photoelectron spectroscopy (ARPES) including spin resolution (SPIN-ARPES) for studies of the electronic structure of solids and surfaces
CoSAXS	3 GeV	Small and wide angle X-ray scattering (SAXS, WAXS) and coherent techniques for soft matter and biomaterials
DanMAX	3 GeV	Powder diffraction (XRD) and full-field tomographic imaging of hard (energy) materials
FemtoMAX	Linac	Time-resolved hard X-ray scattering (XRD) and spectroscopy (XAS) methods for studies of ultrafast processes
FinEstBeAMS	1.5 GeV	Electron and ion spectroscopies and luminescence methodsfor studies of low density matter and solids
FlexPES	1.5 GeV	Soft X-ray spectroscopies for studies of low density matter and solids
ForMAX	3 GeV	Full-field tomography, SAXS/WAXS, scanning SAXS/WAXS imaging
HIPPIE	1.5 GeV	Ambient Pressure Photoelectron Spectroscopy (APXPS) on solids and liquids
MAXPEEM	1.5 GeV	Photoelectron microscopy for investigation of surfaces and interfaces
MicroMAX	3 GeV	Macromolecular crystallography, serial crystallography, time-resolved crystallography
NanoMAX	3 GeV	Imaging with spectroscopic and structural contrast techniques on the nano scale
SoftiMAX	3 GeV	Scanning transmission X-ray microscopy (STXM) and coherent imaging methods
SPECIES	1.5 GeV	Resonant inelastic X-ray scattering (RIXS) and Ambient Pressure Photoelectron Spectroscopy (APXPS)
Veritas	3 GeV	Resonant inelastic X-ray scattering (RIXS) with unique resolving power and high spatial resolution

MAX IV in brief

MAX IV has 16 funded beamline projects at present. The MAX IV accelerator facility performed well in 2020 and delivered X-ray light on schedule and per specification to 14 beamlines, of which 11 received general users and 3 received expert users as part of commissioning activities by year-end. First general users are expected on the latter 3 beamlines by autumn 2021. Construction of the last 2 funded beamlines, ForMAX and MicroMAX, was well along by the end of 2020.

The SARS-CoV-2 pandemic significantly impacted MAX IV beamline operations in 2020, mainly because many users were unable to come to MAX IV for their scheduled beamtime due to travel restrictions. Nevertheless, MAX IV supported experiments by users who could travel to MAX IV as well as a substantial number of user experiments by mail-in services and remote operations. MAX IV updated the user community periodically on these developments and actions taken, including restrictions on visiting, as the Laboratory adapted to the evolving pandemic.

Despite these conditions and with many staff working from home, MAX IV made substantial progress in 2020 on its portfolio of accelerator, beamlines, and other projects, keeping most of them close to schedule. MAX IV completed a long-standing project in 2020 to operate the accelerator facility with a 10 Hz injection rate. FemtoMAX obtained promising early commissioning results demonstrating improved signal-to-noise in diffraction measurements.

The amount and complexity of data produced by MAX IV is growing as the user programme gathers momentum. MAX IV continued development of the KAW-funded DataSTaMP project, which started in July 2019 and runs until July 2024, to implement long-term data storage and data management services at MAX IV.

*Table 1 Number of user visits to´beamlines at MAX IV between 1 March 2020 and 28 February 2021. Beamlines marked with * was baing commissioned.*

Beamline	User visits
Balder	123
BioMAX	464
Bloch	43
CoSAXS	23
DanMAX*	0
FemtoMAX*	0
FinEstBeAMS	21
FlexPES	106
HIPPIE	59
MAXPEEM	48
NanoMAX	82
SoftiMAX*	0
SPECIES-APXPS	57
SPECIES-RIXS	10
Veritas	0
Total	1036

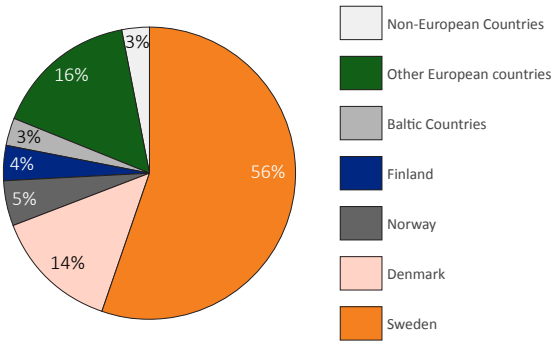


Figure 1 User distribution geographically 1 March 2020 – 28 February 2021

User operations

User programme statistics in this chapter covers the period 1 March 2020 to 28 February 2021, following our proposal schedule. This reporting period coincides with the beginning of the pandemic in Europe. MAX IV was fortunate to be able to continue operating the accelerators and beamlines throughout all of 2020, but the pandemic prevented many users from coming to MAX IV for their scheduled beamtime. MAX IV strived to ensure that as few users as possible lost beamtime due to pandemic issues, and either switched them to some form of remote, mail-in or virtual access where possible or rebooked their experiments.

User statistics for 2020 are not comparable to previous years, in none of the key indicators. The number of submitted and accepted proposals, as well as completed projects was heavily skewed by cancellations, rebooking and carry-over of proposals. Given these caveats, MAX IV hosted 1036 user visits by 560 individual users during this period. The average user gender distribution was 33% women and 67% men. The majority of users (56%) were from Sweden, with most of the rest from other Nordic countries (Figure 1). Other European countries represented 16% and non-European countries represented 14% of the total.

There were three main proposal calls in 2020. The spring call opened in February and closed inMarch was for the period September 2020 to February 2021. 260 proposals were submitted in this call, which included Balder, BioMAX, Bloch, FinEstBeAMS, FlexPES, HIPPIE, MAXPEEM,

NanoMAX, SPECIES-XPS, and Veritas. The autumn call opened in September and closed in October. It was for the period March to August 2021, which included only BioMAX, CoSAXS, DanMAX, SoftiMAX, SPECIES-RIXS, and Veritas, i.e., mainly new beamlines unaffected by a large pandemic backlog. 68 proposals were submitted in this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call. A third merged call opened in December 2020 and closed in February 2021 for the period February 2021 to February 2022. 254 proposals were submitted in this call, which included Balder, Bloch, FemtoMAX 10 Hz, FinEstBeAMS, FlexPES, HIPPIE, MAXPEEM, NanoMAX, SPECIES, and Scanning Probe Microscopy support laboratory.

User meeting

MAX IV hosted the 32nd User Meeting as a digital meeting streamed from the Scandic Star hotel 28–29 September 2020. The 2020 user meeting theme - MAX IV 2020 & 2030 -highlighted the 10-year time frame to go from vision to reality. The theme was a preparation for the development of the MAX IV science-driven strategy.

Young researchers were encouraged to participate in the two MAX IV award competitions. All those who participated were given the opportunity to present their research at the plenary sessions. The awardees were Jalil Shah, for the MAX IV PhD Thesis Award 2020 and Smita Ganguly, for the MAX IV Student Science Award 2020.

The meeting agenda contained facility and user association updates, beamline updates with Q&A, science highlights, keynote speakers and breakout sessions on several different topics. The meeting was wrapped up with a panel discussion and open forum. Each beamline team had prepared a video update recorded at the beamline to share with the participants.

Engaging Industry

Allocation of proprietary beamtime at MAX IV increased during 2020 compared to 2019, in terms of hours sold, number of user organisations involved, and numbers of new beamlines used. In total, 313 hours of proprietary beamtime were sold to 11 different organisations on 43 occasions during 2020.

Two new industrial user groups came in through the Vinnova pilot programme to buy beamtime, and some other groups successfully used the general user programme to access beamtime. The pandemic also affected industrial engagement at MAX IV with cancelled meetings and events, but also in some in unexpectedly positive ways. With most other synchrotrons in the world shutting down or reducing their user programmes, MAX IV was one of the few synchrotrons to turn to experiments. This led to several new industry contacts, particularly within the pharmaceutical industry.

Industrial outreach activities started out strong in early 2020 with a couple of events and meetings. Almost all physical meetings and events abruptly stopped in mid-March due to the pandemic. However, MAX IV hosted a Master Class in the summer on new synchrotron and neutron techniques for the food and packaging sector, through the Northern Lights on Food initiative.

The MAXESS Industry Arena project got traction in 2020 and a website was developed with support funding from Region Skåne. This was launched in the end of October on www.maxess.se.

Collaborations between MAX IV, ESS and SciLifeLab in the life sciences intensified during the year. The joint VR-funded project, InfraLife, will build a hub between the three large-scale research infrastructures to become more accessible to the life science industry and health care sector in Sweden. The project starts in 2021 and runs four years.

Alfa Laval, Lund University and the MAX IV IRO developed a collaboration over the past year to strengthen Swedish and Nordic metal industry connections to MAX IV. Alfa Laval was assigned a full-time position for two years to work closely with the MAX IV IRO.

Collaborations and partnerships
MAX IV collaborated with external partners on several grant applications to various funding agencies in 2020. Some of the major proposals awarded funding, were:

- MAX4MINT, a VR-funded training and education initiative by the User Office and Communications teams to raise the interest of young people in science at MAX IV.
- Four projects (out of nine funded) involving MAX IV through a VR Grant for Accessibility to Research Infrastructure call. The B-branch project, led by Andrey Shivorskiy, is a collaboration involving MAX IV, two Swedish companies, Scienta Omicron and Batteries Sweden, Swerim, and researchers at UU, and LU. B-branch aims to establish a second endstation at HIPPIE dedicated to research on electrochemistry, batteries, energy materials, and corrosion.
- A project titled "Dynamics of proteins in crowded environments on multiple length and time scales," involving the CoSAXS team and researchers at LU, SU and the universities of Siegen and Tübingen in Germany, funded within the Röntgenångström-Cluster. Its aim is to exploit the coherence of the light at CoSAXS in X-ray photon correlation spectroscopy experiments to study protein dynamics.

MAX IV also participated in two major grant proposals within the European landscape that were awarded funding. The first, EC (H2020) – LEAPSINNOV, is a LEAPS pilot project to foster open innovation for accelerator-based light sources in Europe. MAX IV's main contributions to this are leading a networking/co-creation work package and efforts within insertion device development. The second, EC (H2020) – NEP, is a Nanoscience Foundries and Fine Analysis –Europe PILOT project on which MAX IV collaborates with Nanolund. Transnational access to MAX IV facilities is offered through this project. MAX IV is also involved with the Lund Protein Production Platform in a project funded through the European University Alliance for Global Health (EUGLOH) to study the function and structure of SARS-Cov-2 antibodies.

Finance
In 2020, VR, Vinnova, Energimyndigheten, Formas, and 14 Swedish universities including Lund University funded the MAX IV operations budget. The Academy of Finland, DanMAX Consortium, and Vilnius University also contributed.

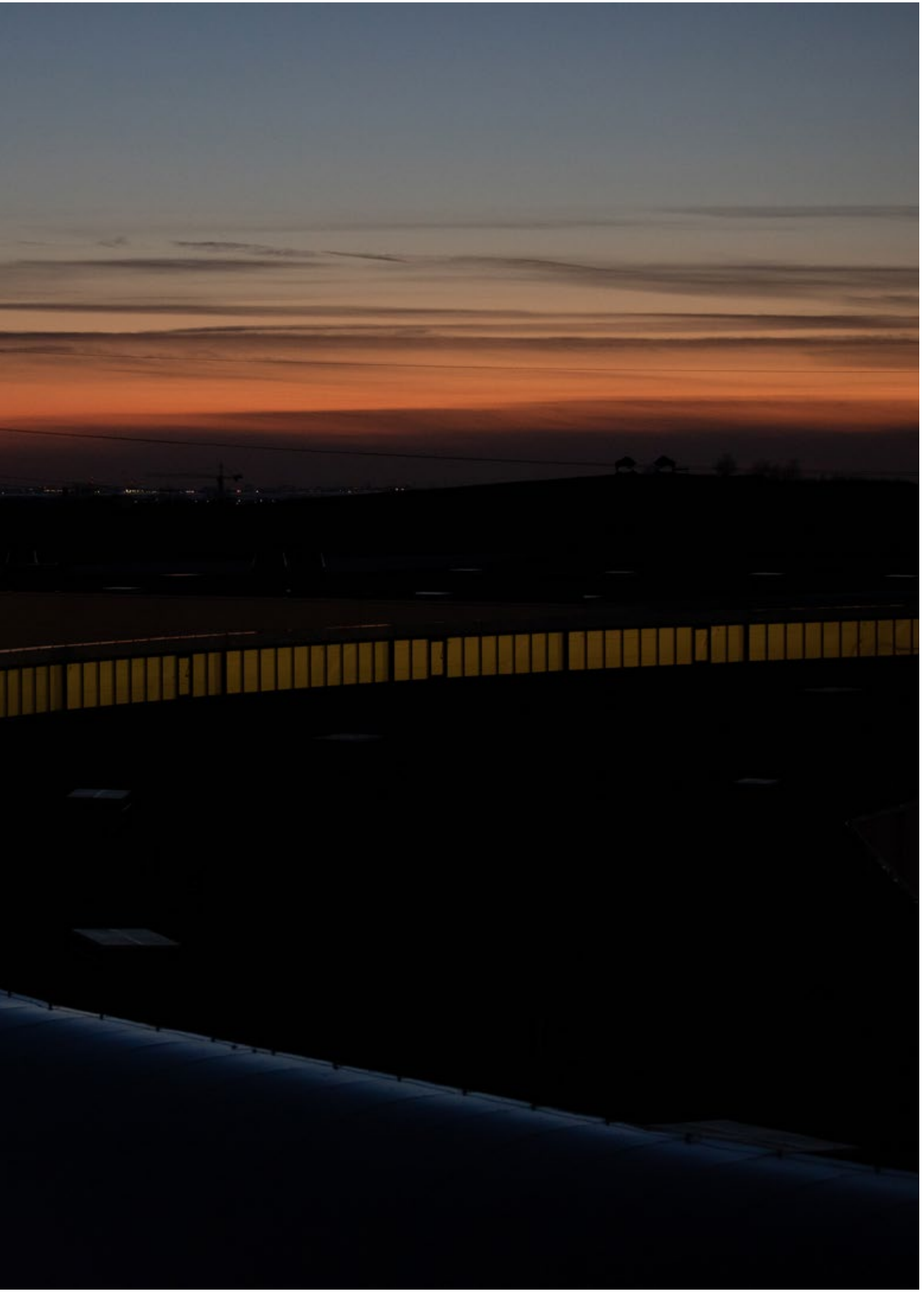
Funding according to the agreement with Swedish universities resulted in a cash contribution of 42 MSEK as income and 8 MSEK in-kind as budgeted.

The total income for proprietary beamtime sales resulted in 1,6 MSEK, with Astra Zeneca accounting for 32% of a total of 10 companies/universities. This industrial engagement is accounted for in more detail above.

As other income, MAX IV accounts for revenue from recycled heat, hosted conferences and guesthouse revenue, some of which was underestimated (+1,2 MSEK).

Organisation and staff
At the end of 2020, MAX IV had 257 employees. Parts of the organisation strengthened by new recruitments included KITS and beamlines, as more beamlines became operational. About one-third of MAX IV employees are from countries other than Sweden. MAX IV advertises most open positions internationally to seek the strongest possible candidates.

Recruitment of a permanent Physical Science Director was initiated in autumn 2020 to fill the position temporarily held by the Interim Physical Science Director, Conny Såthe.



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