FELs OF EUROPE NEWS 1|24

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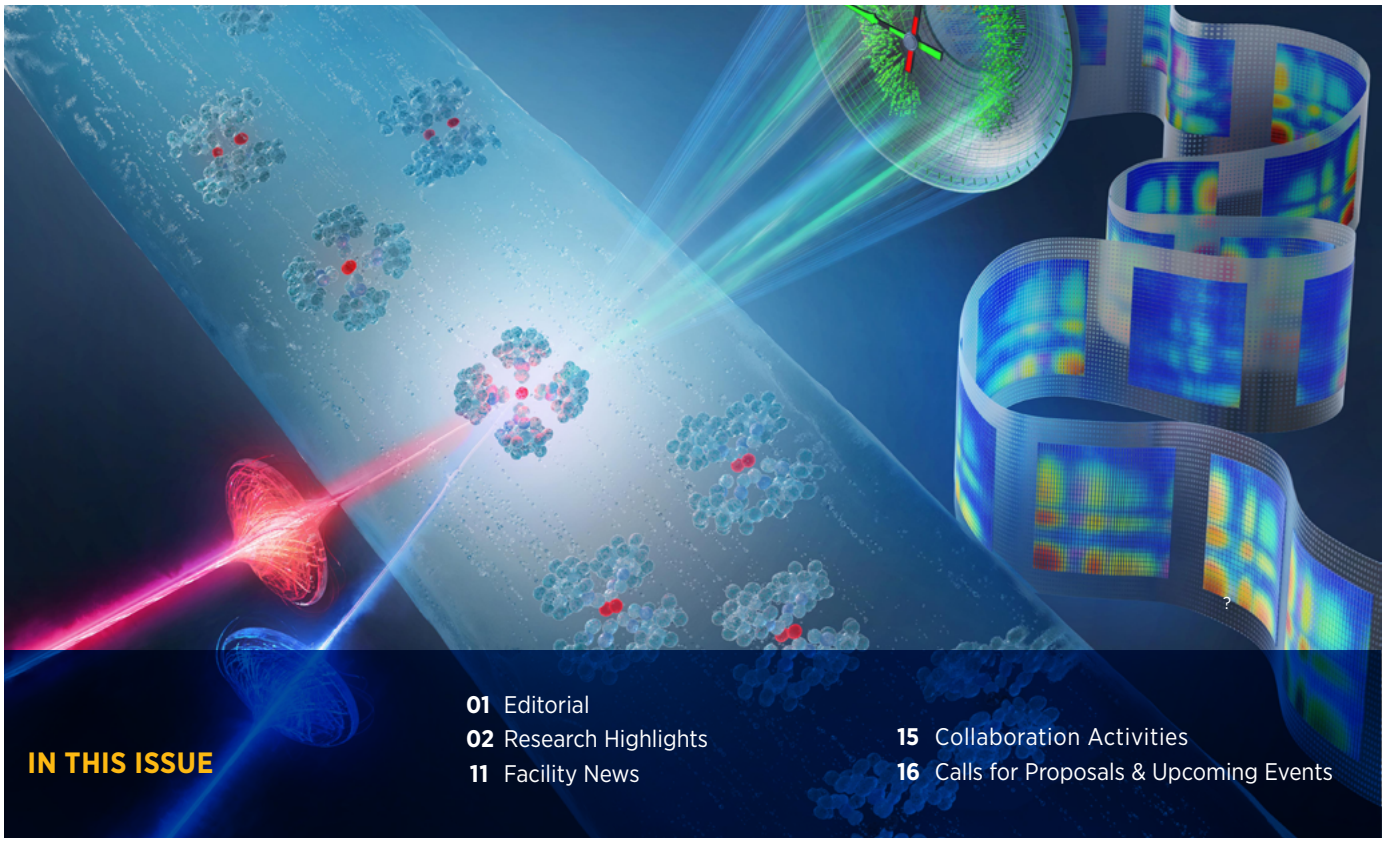


IN THIS ISSUE

EDITORIAL

After some break that was longer than we had hoped for, we are happy to present the first Newsletter of 2024. Quite a few things have to be reported and other things can be announced. To start, our recently established "FELs of Europe Topical Workshop on Selected Problems in FEL Physics: from soft X-rays to THz" was continued with its second edition in Hamburg in November 2023, and it is planned to continue this series in 2025 on a location to be determined soon. Our traditional PhotonDiag workshop took place in Trieste in September 2023 jointly with another event. Last but not least, our "Science at FELs" conference will take place in Paris, June 17-19, 2024, immediately followed by the "Forum on Advanced FEL Techniques".

Our tutorial talks are still taking place roughly every two months, we have a strong and continuous interaction with LEAPS via their Strategy Board and we have contributed to various successful EU project applications. Moreover, one of our members, Britta Redlich from FELIX, became Chair of LEAPS. On the organizational side of FELs of Europe, the management has changed after the two-years period, and the chair's baton was handed over from Serguei Molodtsov to Manfred Helm in the Steering Committee meeting at FELIX, Nijmegen in July 2023. As I write this editorial, I would like to sincerely thank Serguei for his efficient work over the past two years. The Management Board is now completed by Marie-Emmanuelle Couprie and Elke Ploenies-Palm.

With this, we would like to draw your attention to the exciting content of this Newsletter – as usual coming into existence thanks to Britta and the FELIX team as well all contributors – and wish you all a successful year for FELs!

Manfred Helm
Chair FELs OF EUROPE

New applications for “crossed FEL pulses”: beyond EUV transient gratings

The extreme ultraviolet transient grating (EUV TG) approach was initially conceptualized for the coherent excitation of collective modes in condensed matter — such as phonons, magnons, and thermal relaxations — and is now implemented in user-dedicated instruments at FERMI. This groundbreaking method provides a "contact-less" means to explore nanoscale phenomena. Unlike traditional approaches relying on specific sample nanostructuration, the nanoscale sensitivity in EUV TG experiments is not predetermined by the sample's inherent structure. Instead, it is precisely defined by the spatial periodicity of the interference pattern created by two intersecting FEL pulses, as illustrated in Figure 1a.

Probing dynamics in matter at the nanoscale and with ultrafast time resolution holds profound significance for both fundamental science and nanotechnology. However, the core capability of EUV TG instruments, that is the possibility to split and recombine the FEL pulses with large crossing angles and a controllable relative delay, also opens the door to a number of cutting-edge experiments as we point out in the following. Indeed, in this highlight we report how researchers at the FERMI FEL have used the ability to controll “crossed FEL beams” for demonstrating other two types of experimental approaches: (i) three-dimensional (3D) single-shot imaging with sub-100 nm spatial resolution and (ii) frequency-shifted, non-collinear coherent four-wave-mixing (FWM).

In the first case, the two EUV pulses coming from different directions simultaneously hit a 3D object (with reference structures around it), leading to two diffraction patterns that were collected by two CCD cameras; see Figure 1b. Using coherent diffraction imaging algorithms, it was possible to obtain two independent bidimensional images of the sample from the two view angles, and, via a purposely realized ray tracing algorithm, the 3D stereoscopic rendering of the object was retrieved with sub-100 nm resolution; an example is the 5-fold helicoidal structure displayed in Figure 1b. This approach is analogous to depth perception provided by natural binocular vision and “just” need two crossed beams. 3D images can be collected within a single FEL shot, potentially overcoming radiation damage issues and allowing us to use a standard pump-probe approach to detect fast motions of 3D objects.

In the second experiment the EUV TG setup was used in combination with the “twin-seed” mode of the FERMI FEL, which results into a two-pulse train where the wavelength of the two pulses can be independently controlled within a certain range. The two-pulse train was split and precisely delayed before being recombined on a diamond sample, in order to time-overlap the first pulse coming from one side with the second pulse coming from the other side; see Figure 1c. When the wavelength of the first and second FEL pulses is different, their interaction resulted into a grating that “moves” with a velocity proportional to the photon energy difference between the two pulses. This type of interaction is at the basis of many FWM processes that, so far, were limited to optical wavelengths. In this demonstrative experiment the occurrence of a FWM response driven by EUV pulses was revealed by a photon energy shift of a third (optical) pulse. The extension of FWM to EUV and X-ray wavelengths was thoroughly evaluated on theoretical grounds and these results represent a remarkable step forward toward its experimental realization.

The utilization of "crossed FEL pulses" extends beyond extreme ultraviolet transient grating (EUV TG) experiments at FERMI, as researchers have successfully ventured into developing other innovative experiments. Notable among these are: resonant self-diffraction spectroscopy, structured illumination microscopy and transient polarization gratings. These diverse applications highlight the versatility of crossed FEL pulses and their potential to drive advancements in various FEL-based methodologies.

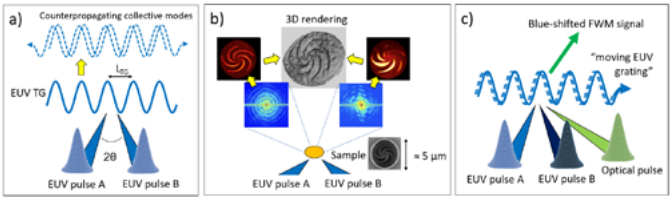


Fig. 1: a) EUV TG excitation. Two EUV pulses of wavelength λ are crossed at the sample with an angle 2θ, generating a transient interference pattern of light intensity (blue wave) with a spatial periodicity $L_{TG}=\lambda/2\sin(\theta)$; the use of EUV wavelengths enables values of L_{TG} in the 10-100 nm range. The EUV TG can launch collective modes at LTG, such as counterpropagating phonons or magnons, sketched as dashed waves. b) Use of crossed EUV pulses for 3D imaging. The two diffraction patterns allow us obtaining high resolution 2D views, as seen by widely different angles (40° in this case; note that the sample was orthogonal to beam B). The 3D structure (shown in greyscale) is finally retrieved by a ray tracing algorithm. c) Moving grating generated by crossed EUV pulses at different photon energies. Its occurrence is probed by a third optical pulse, which interacts with the moving grating through a FWM process, driving the coherent emission of a blue-shifted pulse.

Filippo Bencivenga
Flavio Capotondi
Riccardo Mincigrucci
Claudio Masciovecchio

Original publication:
D. Fainozzi et al., Optica 10, 1053-1058 (2023);
DOI: 10.1364/OPTICA.492730
R. Mincigrucci et al., Optica 10, 1383-1388 (2023);
DOI: 10.1364/OPTICA.497745

Bright and ultrashort X-ray pulses, e.g. for new nuclear clocks

To explore the physical and material properties of samples on the time scale of femtoseconds, scientists need light sources that provide X-rays flashes at very high repetition rate, with short pulse durations and a spectral flux significantly larger than what has been available at X-ray laser sources around the world so far. Using a sophisticated, cascaded Hard X-Ray Self-Seeding (HXRSS) setup, a team led by European XFEL succeeded in generating very bright X-ray flashes at the high repetition rates of the European XFEL accelerator.

The layout of the cascaded HXRSS setup at the European XFEL comprises three undulator segments and two magnetic chicanes with thin diamond crystals. These create a narrow-bandwidth notch in the spectrum, which is then amplified in the subsequent undulator section, resulting in bright X-ray pulses with sharply defined wavelengths.

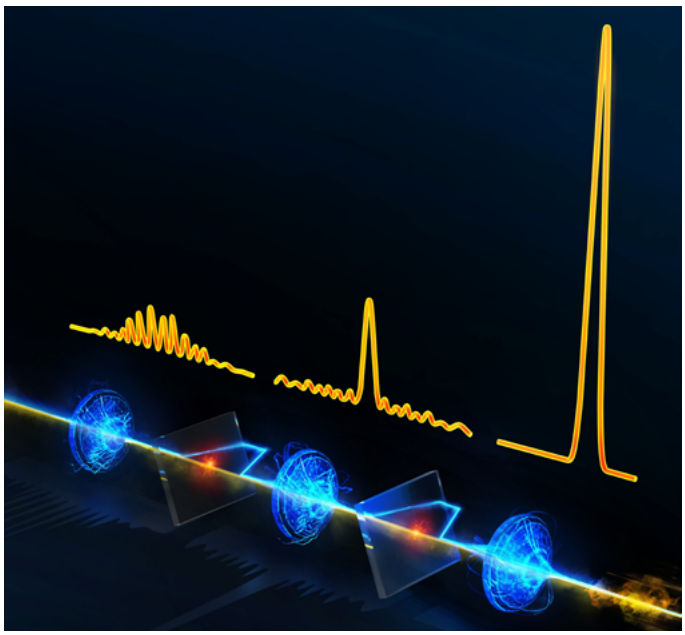


Fig. 1: An artist view of the HXRSS system installed at the European XFEL. Copyright: European XFEL/Tobias Wüstenfeld.

In a conventional HXRSS setup, electron bunches from a linear accelerator generate X-ray radiation in a first undulator section according to the self-amplified spontaneous emission (SASE) scheme. A special filtering process selects only a narrow wavelength range of the radiation, which is then fed as a "seed" into a second undulator section, where it is amplified again. However, due to the high (megahertz) repetition rate of the European XFEL, the diamond crystal that constitutes the main part of the filtering setup heats up, resulting in a shift and a deformation of the range of selected wavelengths.

This unwanted effect was now studied for the first time and demonstrated to be important at X-ray wavelengths longer than 1.5 angstrom. In order to avoid it, an international team of scientists at the European XFEL realized a cascaded setup, where the filtering process is repeated with a second crystal and a final undulator section. In the end, the setup generated thousands of X-ray pulses per second with very narrow spectral bandwidth and an average spectral brightness that was about two orders of magnitude higher compared to any other such X-ray laser facility worldwide.

The HXRSS device opens up exciting new possibilities in a broad range of scientific fields, e.g. for Mössbauer spectroscopy with hard X-ray photons. Such narrow bandwidth can be used for extreme metrology applications with ultraprecise nuclear clocks or to investigate the dynamics and phase transitions in condensed matter. The usage of the HXRSS device at the European XFEL already allowed taking ground-breaking steps toward a new generation of nuclear clocks based on the resonant excitation of the isomer 45Sc. Atomic clocks are currently the world's most accurate timekeepers. Therefore, teams around the world have been working for several years on the concept of a "nuclear" clock, which uses transitions in the atomic nucleus as the pulse generator rather than in the atomic shell. Nuclear resonances are much more acute than the resonances of electrons in the atomic shell used by todays atomic clocks, but also much harder to excite.

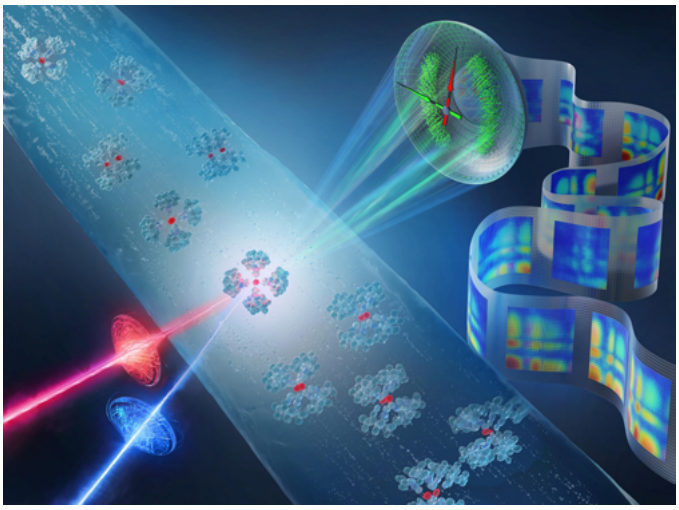


Fig. 2: An artist's rendition of the scandium nuclear clock: scientists used the X-ray pulses of the European XFEL to excite in the atomic nucleus of scandium the sort of processes that can generate a clock signal at an unprecedented precision of one second in 300 billion years. Credit: European XFEL/Helmholtz Institute Jena, Tobias Wüstefeld/Ralf Röhlsberger.

At the European XFEL a team could now excite a promising transition in the nucleus of the element scandium, which is readily available as a high-purity metal foil or as the compound scandium dioxide. This resonance requires X-rays with an energy of 12.4 kiloelectronvolts (keV) and has a width of only 1.4 femtoelectronvolts (feV).

EuXFEL

This corresponds to deviation in counting time of only one second in 300 billion years. The work involved researchers from Argonne National Laboratory in the U.S., the Helmholtz Institute Jena, Friedrich Schiller University Jena, Texas A&M University in the U.S., the Max Planck Institute for Nuclear Physics in Heidelberg, the Polish synchrotron radiation source SOLARIS in Kraków, the European XFEL, and DESY.

References:
"Cascaded hard X-ray self-seeded free-electron laser at megahertz repetition rate", Shan Liu, Christian Grech, Marc Guetg et al., Nat. Photon.
Resonant X-ray excitation of the nuclear clock isomer 45Sc; Yuri Shvyd'ko, Ralf Röhlsberger, Olga Kocharovskaya, et al.; Nature, 2023; DOI: 10.1038/s41586-023-06491-w

European XFEL

PSI

Repairing genetic damage with sunlight

Fig. 1: Photo: Adobe Stock.

DNA damage to the genetic material DNA drives cancer, ageing, and cell death. Therefore, DNA repair is crucial for all organisms, and a deeper understanding of this basic function helps us better comprehend how life around us survives and thrives. An international team of researchers has now revealed how the enzyme photolyase efficiently channels the energy of sunlight into DNA repair chemistry.

All life under the sun must cope with harmful UV rays. UV damage can take many forms, but DNA, the molecule that carries the genetic information of all living organisms, is especially vulnerable. For instance, UV can drive chemical cross-linking reactions of DNA, potentially introducing errors into the genetic code.

This cross-linking can lead to cell death or – in the worst cases – mutagenesis and cancer. Such damage is not uncommon; under bright sunlight, a human skin cell can undergo 50-100 cross linking reactions per second.

"To survive, life has evolved powerful DNA repair mechanisms. One especially elegant solution is provided by the enzyme photolyase," explains DESY scientist Thomas J. Lane, who is also a researcher in the Cluster of Excellence "CUI: Advanced Imaging of Matter" at Universität Hamburg. The enzyme uses sunlight to repair damage caused by sunlight. Photolyase is able to recognize the location where UV irradiation has cross-linked DNA and grabs onto those bits of damaged DNA. Then, it can capture a blue photon from the

sun, and use it to perform repair chemistry, turning the DNA back into its original, healthy form.

Repair enzyme under the SwissFEL microscope

To better understand how photolyase works, the scientists were particularly interested first in the form of the enzyme immediately after absorbing a photon, but before repairing the DNA. Second, they wanted to find out the exact sequence of bond-breaking chemical reactions necessary to turn damaged DNA into healthy DNA. As a third step, the team sought to better understand how photolyase can specifically recognize which DNA is damaged.

Conducting time-resolved crystallography at the SwissFEL X-ray free-electron laser of PSI the scientists were able to capture the excited state of the photolyase chromophore, letting them understand how the enzyme efficiently channels the energy of sunlight into DNA repair chemistry. “This research was only made possible by the recent development of X-ray free-electron laser sources. Their intense femtosecond-duration pulses let us record flash X-ray photographs that freeze all atomic motion so that we can follow the reaction step by step at the speed of molecules,” says first author Nina-Eleni Christou from DESY.

A perfect fit is the key

Further, for decades, it was debated if the two carbon-carbon bonds involved in the repair process broke simultaneously, or in a stepwise fashion. Seeing that one bond breaks first, followed by the second, the team could finally answer this question. Finally, the enzyme has a binding pocket that is perfectly matched to the shape of damaged DNA. The researchers found that the repaired DNA does not fit in this pocket, as it’s too large and has the wrong shape. This explains why photolyase has a higher affinity for the damaged DNA than repaired, healthy DNA.

“This type of experiment is only possible with x-rays from FEL, and exemplifies the capabilities of SwissFEL and Alvra” says Camila Bacellar, group leader and beamline scientist. “We had the opportunity to perform a very similar experiment with another user group as well, where we visualized the repair process by photolyase down to atomic resolution with colleagues from Taiwan. Coincidentally, both these studies have been featured in the same issue of the journal Science, showing the relevance of the results.”

Fig. 2: PSI researcher Camila Bacellar is pleased about the success in precisely analysing the DNA repair enzyme photolyase at the Alvra beamline of the Swiss X-ray free-electron laser SwissFEL. (Photo: Paul Scherrer Institute/Markus Fischer).

The scientists determined ten time-resolved structures of photolyase in the act of DNA repair. “Together, our structures illuminate the function of a powerful DNA repair system that elegantly uses sunlight to repair damage caused by sunlight,” Thomas J. Lane concludes. Unfortunately, humans lack this enzyme and must rely on other DNA repair mechanisms, but photolyase plays an important DNA repair role for nearly all other species.

Text based on a press release by the DESY research centre

Camila Bacellar Cases da Silveira

Original publication:
Time-resolved crystallography captures light-driven DNA repair
Nina-Eleni Christou et al.
Science, 01.12.2023
DOI: 10.1126/science.adj4270
Visualizing the DNA repair process by a photolyase at atomic resolution
Manuel Maestre-Reyna et al.
Science, 01.12.2023
DOI: 10.1126/science.add7795

Tender X-rays show how one of nature's strongest bonds breaks

Fig. 1: New research reveals how the C-H bond – one of the strongest chemical linkages in nature – is easily broken during the C-H activation reaction. (Image: Adobe Stock).

Short flashes of an unusual kind of X-ray light at SwissFEL and SLS bring scientists closer to developing better catalysts to transform the greenhouse gas methane into a less harmful chemical. The result, published in the journal Science, reveals for the first time how carbon-hydrogen bonds of alkanes break and how the catalyst works in this reaction.

Methane, one of the most potent greenhouse gases, is being released into the atmosphere at an increasing rate by livestock farming as well as the continuing unfreezing of permafrost. Transforming methane and longer-chain alkanes into less harmful and in fact useful chemicals would remove the associated threats, and in turn make available a huge feedstock for the chemical industry. However, transforming methane necessitates as a first step the breaking of a C-H bond, one of the strongest chemical linkages in nature.

Forty years ago, molecular metal catalysts were discovered that can easily split C-H bonds. The only thing found to be necessary was a short flash of visible light to "switch on" the catalyst and – baffflingly — the strong C-H bonds of alkanes passing nearby were easily broken almost without using any energy. Despite the importance of this so-called C-H activation reaction, it has remained unknown how that catalyst performs this function. Now, experiments at Swiss FEL and SLS have enabled a research team led by scientists at Uppsala University to directly watch the catalyst at work and reveal how it breaks the C-H bonds.

In their experiments, they triggered the reaction between a rhodium catalyst and an alkane, octane, using an optical laser. Like a high-speed camera, they then used extremely bright and short flashes of X-ray light to take snapshots of the bond breaking process. With this, they could follow the delicate exchange of electrons between the catalyst and a C-H group in octane as it breaks. Discovering the details of this bond breaking process needed two different speeds of flashes. The scientists first used the longer pulses of the SLS to map out the reaction from the beginning to the final C-H bond breaking after 14 nanoseconds. They then used the ultrafast pulses of the SwissFEL to study the initial light-induced activation of the rhodium catalyst that occurs within 400 femtoseconds. The ability — at both SLS and SwissFEL — to access an unusual energy range: the tender X-ray regime is perfectly suited to studying a range of elements — not in the least, rhodium — that play important roles in catalysis, battery research, photovoltaics, biology and environmental science.Tender X-rays lie at a sweet spot between the low energy ('soft') and high energy ('hard') X-rays typically used for research.

There are not many facilities that provide this range because it's difficult to implement and requires extensive modifications of the beamline. These energies are pretty important. They give us access to some elements that are widely available in nature, including sulfur, phosphorous, calcium and also many transition metals. The Phoenix beamline — designed for environmental and chemical science — is tailored to this regime. A mobile pump-probe setup, enables time-resolved measurements, which makes Phoenix the only synchrotron beamline in the world where time resolved X-ray absorption spectroscopy in the tender X-ray range is possible.

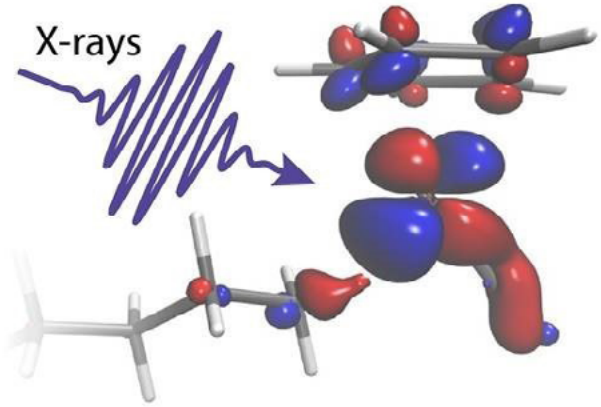


Fig. 2: An X-ray flash illuminates a molecule. (Image: University of Uppsala / Raphael Jay).

Tender X-rays were exactly what was needed to study how the C-H bond breaks in the presence of a metal catalyst, as this range includes the energy absorbed by certain electrons in the rhodium catalyst. "The catalyst is immersed in a dense octane solution, but by taking the perspective of the metal [rhodium], we could specifically pick the one C-H bond out of hundreds of thousands which is made to break," explains Raphael Jay, researcher at Uppsala University and first author of the paper. With the help of theoretical interpretations of their complex experimental data, the scientists could show how electrons were exchanged between the metal catalyst and the C-H group in just the right proportion. "We can see how charge flowing from the metal onto the C-H bond glues the two chemical groups together. Charge flowing in the opposite direction instead acts as a scissor that eventually breaks the C and the H atom apart. The study solves a forty-year-old mystery about how an activated catalyst can break strong C-H bonds by carefully exchanging fractions of electrons without the need for huge temperatures or pressures. The next step will be to learn to direct the flow of electrons to help develop better catalysts for the chemical industry that can make efficient use of methane and other alkanes.

Text: Based on a press release from Uppsala University with additions and modifications from Paul Scherrer Institute/ Miriam Arrell/G. Knopp

Camila Bacellar
Thomas Huthwelker
Grigory Smolentsev
Raphael Jay

Original publication:
Tracking C-H activation with orbital resolution
Jay et al. Science, 1. June 2023 (online)
DOI: 10.1126/science.adf8042

Generating magnetic fields with graphene THz plasmons

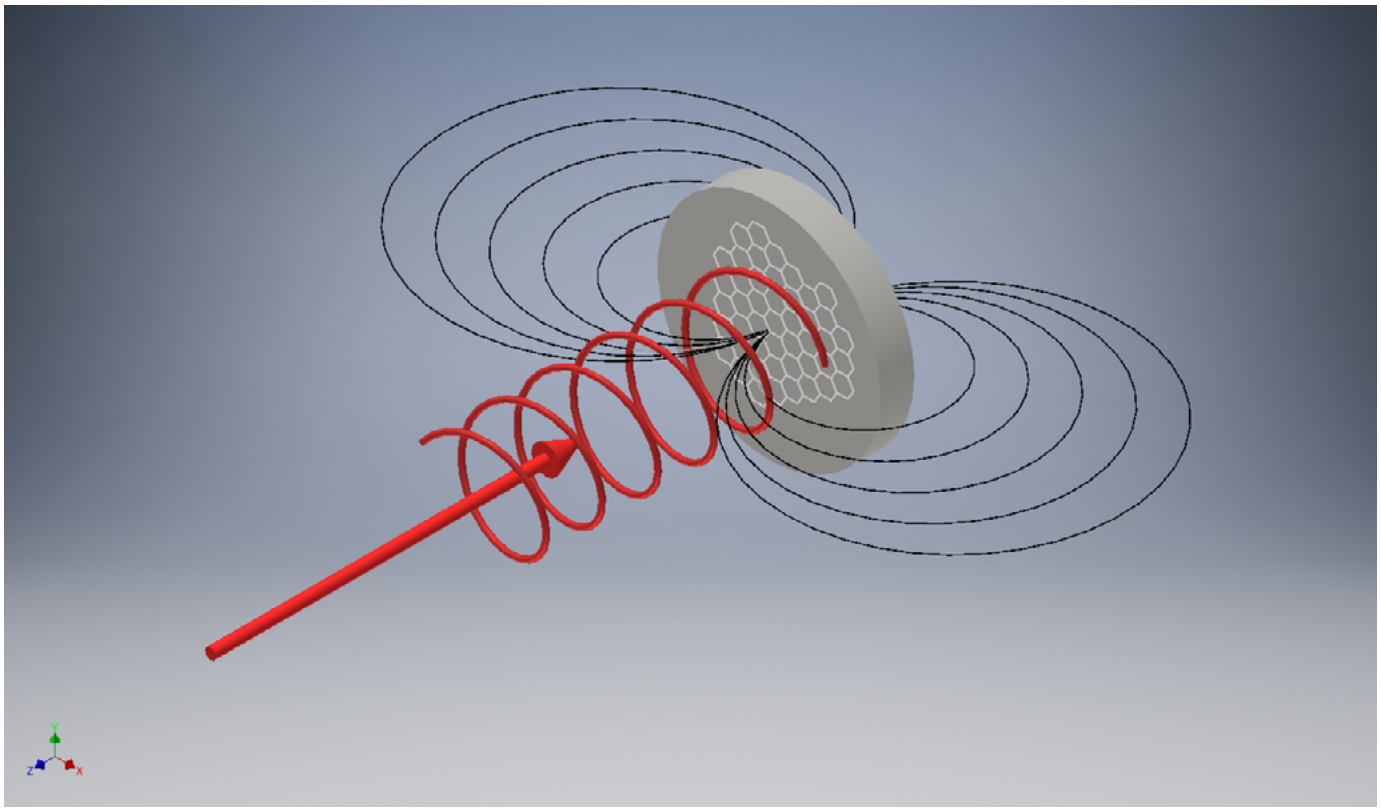


Fig. 1: When a circularly polarized light pulse (red) hits a micrometre-sized graphene disc (grey), a magnetic field is created (black lines). Source: Lucchesi, Uta (HZDR).

Graphene patterned into micrometer-sized disks with sufficiently high carrier density can host localized plasmons. As recent studies have shown, the light-matter interaction strongly increases when the photon frequency is resonant to the plasmon frequency. Such enhancement can increase the efficiency of opto-electronic devices like emitters, modulators, or detectors. In the framework of the collaborative research center CRC1242, funded by the German Research Foundation, we investigated the nonlinear response, utilizing the free-electron laser facility FELBE at Helmholtz-Zentrum Dresden-Rossendorf as a tunable source. In particular, very strong nonlinear transmission changes were observed upon resonant excitation [1]. When a strong THz pulse excites the plasmonic motion of the charge carriers, two main factors lead to a strong decrease of the absorption at resonance: the hot carriers and the strong field enhancement. While the hot carriers lead to a decreased absorption due to a change of the scattering rate and a decrease in chemical potential, the strong localized electric fields also limit the absorption due to the Kerr effect [2].

When linearly polarized THz radiation impinges on the plasmonic structures, the charge carriers oscillate forth and back collectively. When graphene disks are excited by circularly polarized radiation, the plasmonic motion follows the electrical field, resulting in circulating currents. Like in a conventional electromagnet, a quasi-static magnetic field is generated (cf. Fig. 1). In contrast to the magnetic field of the THz radiation, the sign of the magnetic field does not alternate during the field cycle but rather follow the envelope of the THz pulse. The polarity of the magnetic field is determined by the helicity of the THz radiation.

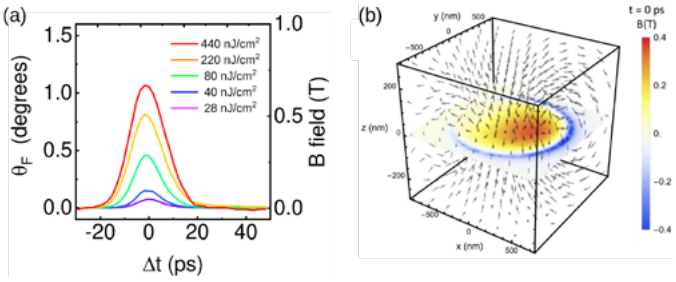


Fig. 2: (a) Pump-induced Faraday roation as a function of the time delay. (b) Calculated field distribution in the vicinity of the graphene disk at the highest pump fluence (taken from [3]).

To investigate this phenomenon, we performed pump-probe experiments at FELBE. The sample consists of quasi free-standing bilayer graphene patterned into a large array of disks with a diameter of 1.2 µm and a periodicity of 1.5

While circularly polarized pump pulses excite the circular plasmons, Faraday rotation of linearly polarized THz radiation was exploited to probe the magnetic field in the disks. A wire-grid polarizer served as polarization-dependent beam splitter, two bolometers measured the transmission as a function of the time delay between pump and

probe pulse. When excited with a moderate fluence of about 440 nJ/cm^2 we observed a maximum change in polarization of about 1°. A comparable Faraday rotation is reached in a static magnetic field of about 0.5 T. Considering the thickness of the bilayer graphene, this corresponds to a Verdet constant of about 5·10^7 rad/(T m). As the temporal development of the magnetic field is directly linked to the plasmon lifetime in graphene, the duration of the pump-induced magnetic field is determined by the pulse duration of FELBE (cf. Fig. 2(a)).

As the magnetic field is caused by the circulating plasmon, the field distribution is not homogeneous throughout the disks. To further analyze this, we performed finite-element simulations of the graphene disks when excited by circularly polarized radiation with the highest field strength applied in the experiment. As can be seen in Fig. 2(b), the area of the strongest magnetic field is bound to the strongest currents caused by the plasmons. Such disks of plasmonic elements might be exploited in future for ultrafast control of magnetic fields with THz radiation.

Martin Mittendorff

References:
[1] M. M. Jadidi, K. M. Daniels, R. L. Myers-Ward, D. K. Gaskill, J. C. König-Otto, S. Winnerl, A. B. Sushkov, H. D. Drew, T. E. Murphy, and M. Mittendorff, "Optical Control of Plasmonic Hot Carriers in Graphene," ACS Photonics 6, 302 (2019).
[2] J. W. Han, M. L. Chin, S. Matschy, J. Poojali, A. Seidl, S. Winnerl, H. A. Hafez, D. Turchinovich, G. Kumar, R. L. Myers-Ward, M. T. Dejarld, K. M. Daniels, H. D. Drew, T. E. Murphy, and M. Mittendorff, "Plasmonic Terahertz Nonlinearity in Graphene Disks" Adv. Photonic Res. 3, 2100218 (2022).
[3] J. W. Han, P. Sai, D. B. But, E. Uykur, S. Winnerl, G. Kumar, M. L. Chin, R. L. Myers-Ward, M. T. Dejarld, K. M. Daniels, T. E. Murphy, W. Knap, and M. Mittendorff, "Strong transient magnetic fields induced by THz-driven plasmons in graphene disks," Nat. Commun. 14, 7493 (2023).

FELIX Laboratory

New analytical methods coupled with FELIX used to identify biomarkers for GLUT1DS

Researchers at the HFML-FELIX laboratory (Radboud University), Synthetic Organic Chemistry (Radboud University), the Translational Metabolic Laboratory (Radboudumc), Bruker (Bremen, DE) and Janssen Pharma (Beerse, BE) have developed a combined analytical methodology to distinguish the structures of oligosaccharides – complex biomolecules that play crucial roles in a host of essential biological functions. Using this novel approach, they have analysed the cerebrospinal fluid (CSF) of patients with glucose transporter type-1 deficiency syndrome (GLUT1DS) and identified two novel biomarkers for the disease.

Mass spectrometry (MS)-based technologies combined with orthogonal separation techniques, in many cases liquid chromatography (LC), are a cornerstone of the modern analytical sciences. These techniques are tremendously sensitive but lack the structure-diagnostic capabilities of spectroscopic techniques such as NMR and infrared spectroscopy. Therefore, distinguishing isomeric molecules can often be challenging using LC-MS based approaches. In contrast, infrared ion spectroscopy (IRIS) can be used to identify molecular structures detected in mass spectrometry (MS) experiments based on their vibrational spectra. The direct coupling of LC and IRIS is challenging due to the mismatching timescales of the two

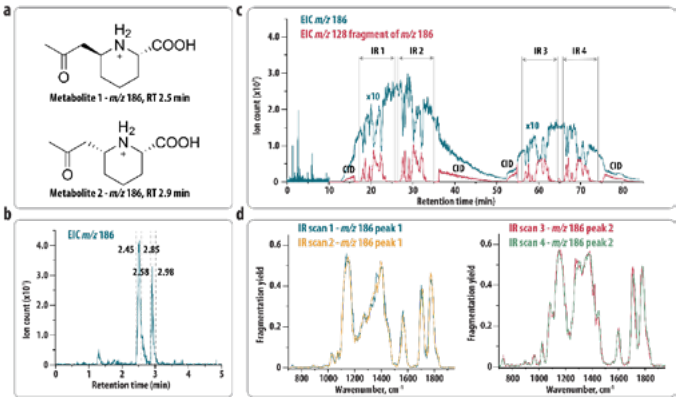


Fig. 1: Two closely related isomers are separated using LC, but only elute for ~13 seconds each (left panel). Using the novel LC-IRIS approach described above, it was possible to measure in duplicate the IR spectra of each LC-separated isomer allowing their identification.

experiments: an IRIS experiment typically takes several minutes, whereas an LC fraction elutes in several seconds. In a recent study published in the journal Analytical Chemistry [1], the researchers developed a new approach combining LC and IRIS, utilizing two switching valves and two sample loops as an alternative to direct online LC-IRIS coupling, giving extended analysis times.

FELIX Laboratory

In a proof-of-concept demonstration of the sensitivity, multiple IR spectra were recorded of retention time and m/z separated compounds present in a 2 µL sample at µM concentration.

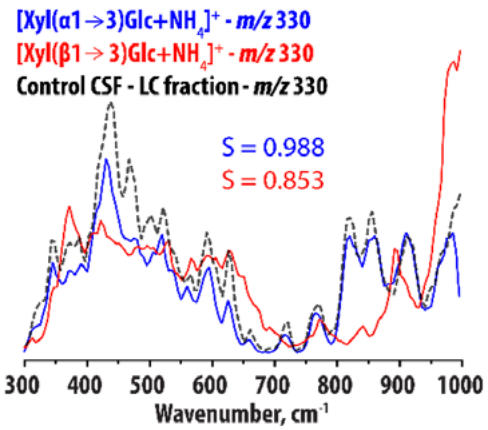
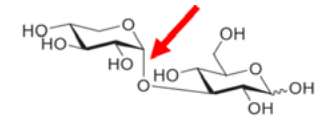
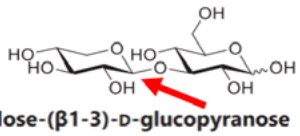


Fig. 2: An unknown molecular feature was absent in the CSF of GLUT1DS patients while present in the CSF of non-patients. Tagging the metabolite with NH4+ and recording its far-infrared spectrum using FELIX, the molecular structure was identified as D-xylose-(**α**1-3)-D-glucopyranose. The IR spectra are sufficiently distinct to discriminate this structure from the (β1-3) isomer.

Until recently, it was thought that saccharides pose a unique challenge for analysis using IRIS due to their high conformational flexibility and extensive intramolecular hydrogen bonding that typically leads to infrared spectra with broad and unresolved features in the vibrational fingerprint region (1000-4000 cm^{-1}) at room temperature, typically lacking diagnostic value for the identification of closely related isomers. In a second study published in Analytical Chemistry [2], the researchers demonstrate another novelty by introducing the previously unexplored far-infrared range (250–1000 cm^{-1}), finding well-resolved and highly diagnostic features for ion-complexed oligosaccharides. This enables the distinction of isomers, differing by their composition of monosaccharide units and/or their glycosidic linkages, up to the size of tetrasaccharides. The combination of this method with hydrophilic interaction liquid chromatography (HILIC) was applied to identify novel biomarkers of GLUT1DS[3].



D-xylose-(α1-3)-D-glucopyranose



D-xylose-(β1-3)-D-glucopyranose

Two previously unknown oligosaccharides were identified in cerebrospinal fluid that are suspected to originate from glycosylated proteins, potentially improving diagnostics as well as our pathophysiological understanding of the disease. Their decreased levels in GLUT1DS patients are hypothesized to be a consequence of insufficient glucose and suggest that glucose deficiency in GLUT1DS may cause disruptions that go beyond energy metabolism.

Jonathan Martens
Jos Oomens

References:

[1] Rianne E. van Outersterp, Jitse Oosterhout, Christoph R. Gebhardt, Giel Berden, Udo F. H. Engelke, Ron A. Wevers, Filip Cuyckens, Jos Oomens, and Jonathan Martens, Targeted Small-Molecule Identification Using Heartcutting Liquid Chromatography–Infrared Ion Spectroscopy, Analytical Chemistry, 2023, 95 (6), 3406-3413 DOI: 10.1021/acs.analchem.2c04904

[2] Rianne E. van Outersterp, Pieter C. Kooijman, Jona Merx, Udo F.H. Engelke, Nematollah Omidikia, Mei-Lan H. Tonneijck, Kas J. Houthuijs, Giel Berden, Tessa M.A. Peters, Dirk J. Lefeber, Michel A. A. P. Willemsen, Jasmin Mecinovic, Jeroen J. Jansen, Karlien L.M. Coene, Ron A. Wevers, Thomas J. Boltje, Jos Oomens, and Jonathan Martens, Distinguishing Oligosaccharide Isomers Using Far-Infrared Ion Spectroscopy: Identification of Biomarkers for Inborn Errors of Metabolism, Anal. Chem., 2023 95 (26), 9787-9796 DOI: 10.1021/acs.analchem.3c00363

[3] Tessa M. A. Peters, Jona Merx, Pieter C. Kooijman, Marek Noga, Siebolt de Boer, Loes A. van Gemert, Guido Salden, Udo F. H. Engelke, Dirk J. Lefeber, Rianne E. van Outersterp, Giel Berden, Thomas J. Boltje, Rafael Artuch, Leticia Pías-Peleteiro, Ángeles García-Cazorla, Ivo Barić, Beat Thöny, Jos Oomens, Jonathan Martens, Ron A. Wevers, Marcel M. Verbeek, Karlien L. M. Coene, Michèl A. A. P. Willemsen. Novel cerebrospinal fluid biomarkers of glucose transporter type 1 deficiency syndrome: Implications beyond the brain's energy deficit. J. Inherit. Metab. Dis., 2023; 46(1): 66-75. doi:10.1002/jimd.12554

Looking back at a successful year 2023, and looking forward into 2024 with new Chairman Thomas Feurer

Fig. 1: Prof. Thomas Feurer, Copyright: private

With more than 1,200 users from over 30 countries completing 89 experiments at the facility in 2023 European XFEL looks back at yet another successful year of user operation. Despite the challenges caused by the war in Ukraine, European XFEL met its objectives by further improving the scientific opportunities for experiments, and, together with DESY further improved the performance of its superconducting accelerator, which is currently serving seven experiment stations at three SASE beamlines.

In January 2024, European XFEL also completed the planned change in the Management Board, with Thomas Feurer assuming the role of the new Chairman of the European XFEL Management Board on 1 January. Hailing from the University of Bern, Feurer is the successor to Prof. Robert Feidenhans'l. Feidenhans'l had held the position since January 2017 and will continue as an advisor until his retirement in July 2024.

Feurer's research areas in Bern included laser physics, ultrafast spectroscopy and the development of instruments for research on X-ray lasers such as the European XFEL. He previously worked as a researcher at the Massachusetts Institute of Technology (MIT) for several years and studied physics at the Universities of Würzburg and Jena. During the past six months Feurer has already been involved in the development of the 2030 Strategy process of the European XFEL and has contributed with important insights.
On behalf of the European XFEL Council, Federico Boscherini warmly thanked Robert Feidenhans'l for his extraordinary contribution to European XFEL. "As one of my predecessors as Chairman of the Council, Robert was a key figure in the planning and construction of the facility. Later, as Chairman of the Management Board, he successfully guided the facility through the first years of user operation and set the course for the future with the development of the Strategy 2030," said Boscherini.

The European XFEL Management Board consists of two Managing Directors, Prof Thomas Feurer and Dr Nicole Elleuche, as well as the Scientific Directors Prof Serguei Molodtsov, Dr Sakura Pascarelli and Dr Thomas Tschentscher.

In July 2023 the European XFEL control software Karabo was released as open source. The European XFEL control system has been developed into a modern, distributed software framework that enables control and monitoring of the photon systems and instrumentation at the facility, as well as data acquisition from X-ray detectors capable of megahertz frame rates. It is highly interoperable with DOOCS, a similar system developed at DESY that is used

to control the European XFEL accelerator. Karabo is highly scalable – it can run on a small system on a chip such as a Raspberry PI or on a system with tens of computing cores. At the European XFEL, the Karabo control system handles about 3.7 million control parameters on 30 000 devices over 13 major installations. Karabo is available via www.karabo.eu.

The Diode Pumped Optical Laser for Experiments (DiPOLE), is a new type of laser that can generate high-energy bursts of green light very efficiently. Developed by scientists at the Science and Technology Facilities Council's Central Laser Facility (CLF) in the UK in the framework of the HiBEF user consortium, the laser can deliver up to 10 high energy pulses per second. These powerful pulses are just a few nanoseconds long, and can be used as a 'hammer' to create intense shock-waves in different types of matter. DiPOLE's high-energy pulses enables to create conditions with pressures of up to 10 000 tonnes per square centimeter and temperatures above 10 000 degrees in a very short time allowing scientists to create states of matter that only exist on distant exoplanets or deep within the interior of the Earth.

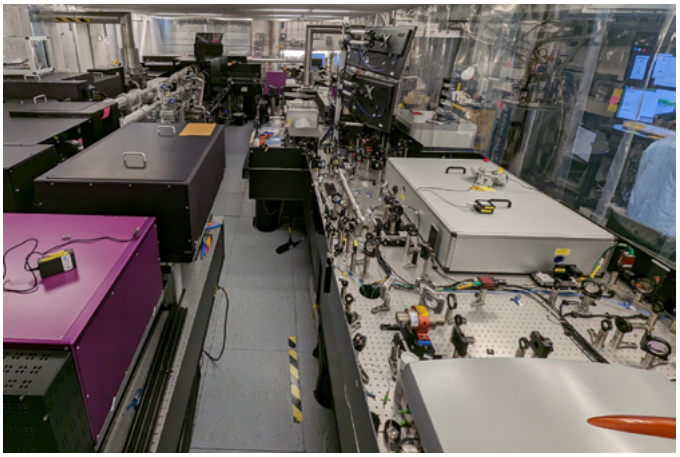


Fig. 2: The new DiPOLE laser at the HED experiment station. Copyright: HZDR.

European XFEL has also developed a comprehensive set of Open Educational Resources on virus research aimed at senior high school students. These materials, developed as part of a Joachim Herz Foundation-funded initiative, comprise four distinct modules covering various facets of virus research and can be utilized either collectively or individually in classrooms and school laboratories. Furthermore, the material will be used in the Xcool Lab at European XFEL, which is currently under construction, after the opening of the lab in autumn 2024.

The modules include an informative and entertaining short movie highlighting virus research, an experiment dedicated to identifying coronavirus variants, materials for DNA sequencing and the design of essential primers crucial for DNA amplification. The resources are now freely accessible in English or German as Open Educational Resources (OER) under a Creative Commons license. Through engaging materials and hands-on activities, the European XFEL aims to inspire the next generation of researchers.

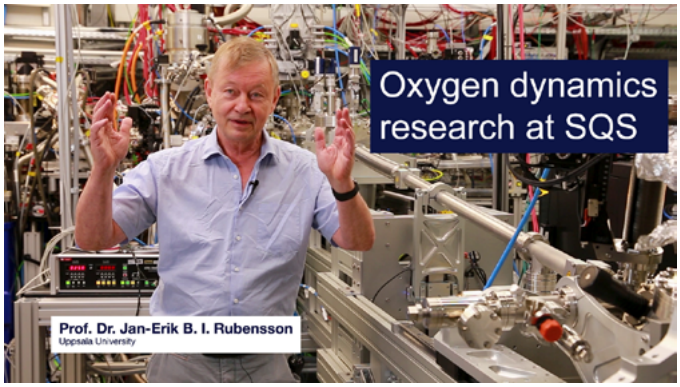


Fig. 3: Jan-Eric B. I. Rubensson from Uppsala university explaining the EuXFEL SQS instrument.

Last but not least European XFEL presents a new series of captivating videos featuring scientists shedding light on their experiments at the facility. The videos take viewers on a journey to the European XFEL instruments. They offer a fascinating glimpse into the experiments. Everybody is invited to explore additional videos available in the playlist https://www.youtube.com/@EuropeanXFEL.

Gerhard Samulat

Status of Installation and Commissioning at TARLA-FEL Facility

In 2023, the installation and commissioning activities in TARLA-FEL facility continued with increasing intensity. Two largest auxiliary systems of TARLA accelerator, namely helium refrigeration plant and water-cooling plant, were completed and commissioned. After the successful commissioning of the cryogenic system, cryomodules were cooled down to 1.8 K and high-power RF conditioning started in December 2023. The very first superconducting cavity reached to its design accelerating gradient of 12.5 MV/m on 12th December. RF conditioning was paused due to a problem in helium refrigeration plant, but will restart in February 2024. The installation of the injector beamline was completed and its beam commissioning started. It is foreseen to connect the injector beamline to the first cryomodule in March 2024 and demonstrate acceleration through the first cryomodule in April. A picture of the injector and the first cryomodule inside the accelerator hall can be seen in Figure 1.

Fig. 1 Picture showing the injector beamline and the first cryomodule of TARLA electron accelerator.

Fig. 2: M1 of the optical cavity.

Fig. 3: M2 of the optical cavity.

In addition to the accelerator beamline and auxiliary systems, the optical cavity for the undulator with 35 mm period length was assembled and its mechanical tests were successfully completed. The optical cavity was designed and assembled at TARLA. The technology group is currently performing the performance tests of the system. Initial results already showed that the stability of the system is below 100 nrad (1 sigma) with resolutions for tilt angle below 50 nrad. Figures 2 and 3 show the M1 and M2 systems of the optical cavity in the FEL hall.

Veli Yıldız

UK XFEL User Engagement Campaign

Fig. 1: Speakers and organisers of the UK XFEL Townhall at the University of Plymouth.

Momentum is building around the UK XFEL project, which is staging a series of Townhall meetings around all parts of the UK to engage the community in plans for access to next-generation XFEL capability. It is envisaged that a next-generation XFEL would deliver a step-change increase in the number of simultaneous experiments, together with developments to enhance the already unique capabilities of XFELs. These Townhall meetings set out to discuss the details of these capabilities along with the possible science that could be carried out on such a facility, it has therefore been important that the meetings encompass a wide spectrum of the scientific and industrial community, not just those who currently use XFELs. To develop this idea, and promote discussion, a number of non-XFEL users have already been invited to talk about how they could use such a next-generation XFEL.

Led by the Science and Technology Facilities Council, the UK XFEL project is now a year into a three-year Conceptual Design and Options Analysis, supported by the UK Research and Innovation Infrastructure Fund. By the end of 2025 the project team will have evaluated the conceptual design of a new facility based in the UK, as well as assessing alternative options for UK users gaining access to next-generation XFEL capabilities by investing at existing international facilities.

Each Townhall meeting is a two-day event, starting with an opening talk aimed at giving an overview of the project, updates on the facility design and a review of XFEL science, before moving on to more focused science and technology themes. The series started in June 2023 at Queen's University Belfast, with a focus on the frontiers of measurement technology. This was followed by an event at the University of Strathclyde, Glasgow, in October focused on materials, chemistry and biology at extreme conditions.

The latest event was held at the University of Plymouth in January 2024, to discuss the benefits that a next generation XFEL could bring to quantum computing, AI applications and fundamental physics. With these themes, it was a fitting first international meeting to be held in Plymouth's brand new Babbage building, named in honour of Charles Babbage for his transformative breakthroughs in computing. As at both previous Townhalls, there was a vibrant set of talks and discussions, with numerous ideas to utilise the proposed features of a next-generation XFEL, how the fundamental physics community need to engage early to help shape the design, and potential novel acceleration techniques which could be deployed at a FEL. Discussions around the data requirements of such a facility and how it can be impacted by the AI/machine learning community were also highlighted during the sessions. The first day was closed by our keynote speaker, Professor Sir Peter Knight who delivered an insightful talk explaining how the UK has recently developed a national strategy for quantum technology.

A further four Townhall events are planned for 2024, with the next being hosted by the Diamond Light Source at the Rutherford Appleton Laboratory in Oxfordshire, with a focus on Life Sciences. The project team encourages everyone interested to join either in person or online – details will be released via the project website and mailing list (https://xfel.ac.uk/).

Jim Clarke

Science@FELs 2024

Synchrotron SOLEIL and Sorbonne University (Paris) invite you to join the Science at FELs conference, June 17-19, 2024 and the Forum on Advanced FEL Techniques, June 20-21, 2024. After the previous successful meeting in Hamburg and the exciting new developments and results from these extraordinary light sources, we are looking forward to a fascinating and informative conference. The meeting will include the hottest new results, of course, but also tutorials on the operation and uses of FEL radiation along with possible tours of relevant accelerator and laser-based sources in the Paris-Saclay area (SOLEIL beamlines, CLIO infra-red FEL, ATTOLAB, APOLLON laser facility, Laser Plasma Acceleration at LOA). The one and a half day "Forum on Advanced FEL Techniques", aiming to bring together FEL experts and FEL users, will take place right after the main conference.

For further information, please check the conference website: https://www.synchrotron-soleil.fr/en/events/sciencefels-2024

Registration are open on until May 13 th (late registration) and April 8 th (early registration): https://indico.synchrotron-soleil.fr/event/59/

Synchrotron SOLEIL and Sorbonne University (Paris) are looking forward welcoming you in June for the Science@FELs 2024.

Workshops 2023

The 6th PhotonDiag workshop took place from 12-14 September 2023 in Trieste. This year the PhotonDiag workshop was merged with the "MEADOW – 10 years after", celebrating the 10th anniversary of the "MEtrology, Astronomy, Diagnostics and Optics Workshop". The next PhotonDiag Conference is planned to take place 2025 as a face-to-face meeting in the UK. The "FELs of Europe Topical Workshop on Selected Problems in FEL Physics: from soft X-rays to THz" was continued with its second edition from 14-17 November 2023 in Hamburg. The event was followed by a satellite meeting, focusing on the topic of advanced synchronization systems.

About FELs of Europe

FELs OF EUROPE is an initiative of the ESFRI projects EuroFEL and European XFEL. It is a collaboration of all free electron laser (FEL) facilities in Europe, with the goal to meet technological and scientific challenges of these novel and rapidly developing technologies, and to provide a worldwide unique, pan-European research infrastructure that enables exploiting the full scientific potential of these unique accelerator based short-pulse light sources. The collaboration includes 14 facilities in 10 countries.

All members are either operating or developing free electron laser (FEL) facilities and/or advanced short-pulse light sources (SPS), based on accelerator technologies. Due to their unique properties, these light sources provide a step change in the ability to address research needs across the disciplines of physics, chemistry, materials, and life sciences. FELs will improve our understanding of processes on a molecular level, leading to development of new materials and methods for tomorrow's technological advancement, clean environment, sustainable energy, and health care.

FELs OF EUROPE will facilitate the enhancement and exploitation of the full scientific potential of FELs in an efficient way by promoting joint technical development and collaborating closely with users and related communities. It will promote efficient open access to the research infrastructure and optimal conditions for users.

More info at: www.fels-of-europe.eu

CURRENT AND UPCOMING CALLS FOR PROPOSALS

www.fels-of-europe.eu/user_area/call_for_proposals

For experiments at FERMI
Deadline: 31 May 2024
For experiments at FELBE
Deadline: 23 Sept. 2024
For experiments at FELIX
Deadline: deadline 15 May 2024
For experiments at SwissFEL
Deadline: 15 Sept. 2024

UPCOMING EVENTS

Science@FELs Conference — organized by Soleil and Sorbonne University
17-19 June 2024
https://www.synchrotron-soleil.fr/en/events/sciencefels-2024

Forum on Advanced FEL Techniques — Satellite workshop
20- 21 June 2024

The next PhotonDiag Conference will take place 2025 in UK, further details will be published in due time

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