Dnr: STYR 2022/368

Annual Report
MAX IV Laboratory

2021

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1 In Brief

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

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

The scientific output of the laboratory continues to grow. In 2021, and at the time of the writing of this report, users and staff reported 138 articles in peer-reviewed journals. This is a 34% increase as compared to 2020. The scientific impact of the research done at MAX IV is high, with an average impact factor of $\langle IF \rangle = 7.1$. More than one third (37%) of the 2021 articles were published in journals with an impact factor larger than the average impact factor $\langle IF \rangle$.

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

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

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

2 Scientific Output

All 2021 MAX IV laboratory publications are listed in detail in Appendix 5 and are available on our website at: https://www.maxiv.lu.se/science/publications/.

At the time of writing this report and for 2021, the MAX IV laboratory publication database contained 138 peer-reviewed articles, as indicated by the dotted line in Figure 1. This corresponds to a 34% increase compared to 103 and 102 publications in 2020 and 2019, respectively.

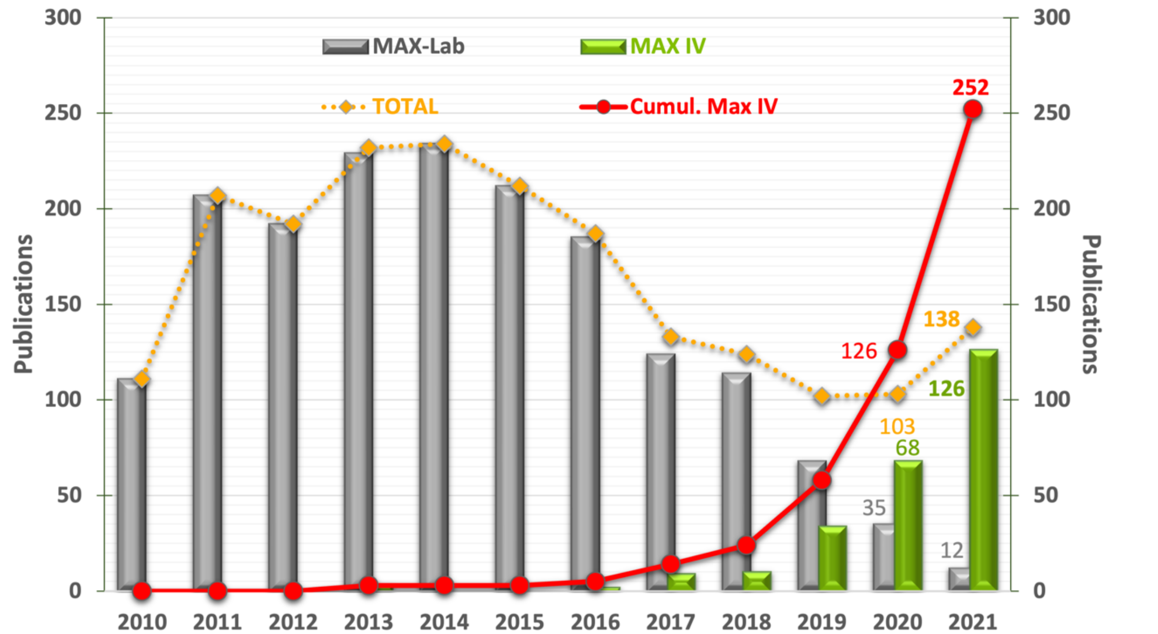

Figure 1: Histogram: the number of publications per year discussing data measured at MAX-Lab and MAX IV in gray and green, respectively. The dotted line indicates the total number of publications per year (MAX IV and MAX-Lab). The solid line displays the cumulative number of MAX IV publications.

The total number of publications contains articles data measured at MAX-Lab in gray and MAX IV in green. Publications that use data measured both at MAX-Lab and MAX IV are counted as MAX IV. Publications discussing data measured at MAX-Lab only continue to decline since 2014 (gray histogram), i.e., a 66% decrease from 2020. In contrast, MAX IV data (green histogram) continues to increase and shows an 85% increase in comparison to 2020.

Since 2020, the number of publications using data from MAX IV surpasses the one containing data measured at MAX-Lab. This is, for example, highlighted in Figure 2, for which 9% of the

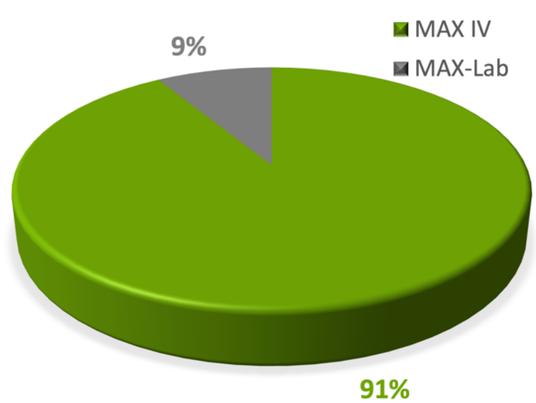

Figure 2: Distribution of 2021 publications involving measurement at MAX IV & MAX-Lab. Data measured both at MAX IV and MAX-Lab are considered MAX IV.

publications refer to data measured solely at MAX-Lab. We expect this diminution of MAX-Lab publications to continue.
The cumulative number of MAX IV publications, as indicated with the solid line in Figure1, increases with 252 publications in 2021, a 100% increase as compared to 2020. This is consistent with the increasing number of beamlines transitioning to user operation (i.e., thirteen (13) by December 2021) and the increased capabilities of individual beamlines. We expect this trend to continue. We also note that ten (10) PhD or MSc theses were completed in 2021 using results obtained at MAX IV.
A graphical representation of the scientific impact of the work performed at MAX IV is presented in Figure 3. It displays the histogram of the 2021 publications frequency as a function of the journal impact factor (i.e., Clarivate, 2020). We note the following:

- The average impact factor of all publications in 2021 is ⟨IF⟩ = 7.1
- Nearly 35% of our publications are in journals with an impact factor larger than the average impact factor ⟨IF⟩ = 7.1, indicated with the dash-dotted line in Figure 3.
- We note that three publications are in journals with an impact factor above 20: Advanced Energy Materials, Nature Electronics, and Science.

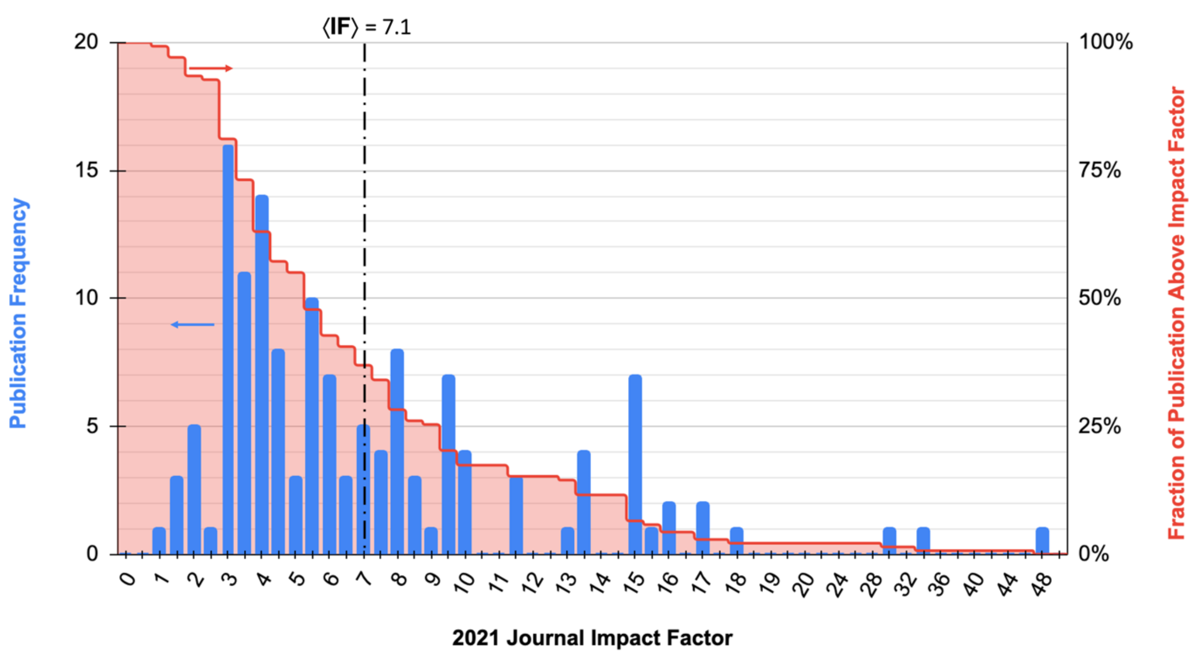

Figure 3: Histogram and left axis: Publications frequency as a function of the 2020 journals impact factor (IF). Solid line and right axis: Fraction of 2021 publications above a specific journal impact factor IF. The dash-dotted line indicates the average impact factor ⟨IF⟩ = 7.1.

Figure 4 presents the distribution of peer-reviewed publications related to data measured before 2016 at MAX Lab (yellow), among our MAX IV beamlines (green), and the ones associated with the development of our accelerator complex (blue). Publications connected to data measured at MAX-Lab and MAX IV are credited to the respective MAX IV beamline. Beamlines are ordered by when they were introduced to user operation from top to bottom. We note the following:

- In 2021, twelve (12) publications were related to data measured at MAX-Lab before 2016 and did not involve any of the MAX IV beamlines.
- The large productivity of the BioMAX beamline with 38.5 publications (not to scale). BioMAX is our beamline providing the life sciences user community with high-throughput macromolecular crystallography. Its high level of automation fully supports mail-in and remote experiments. These features became critical in ensuring the continuation of its user program during the Covid-19 pandemic.
- Some of our beamlines are reaching a certain level of maturity in developing their user program after several years of commissioning. This is, in particular, the case for our soft and hard X-ray spectroscopy beamlines (BLOCH, HIPPIE, FinEstBeMS, BLOCH, FlexPES, and SPECIES).

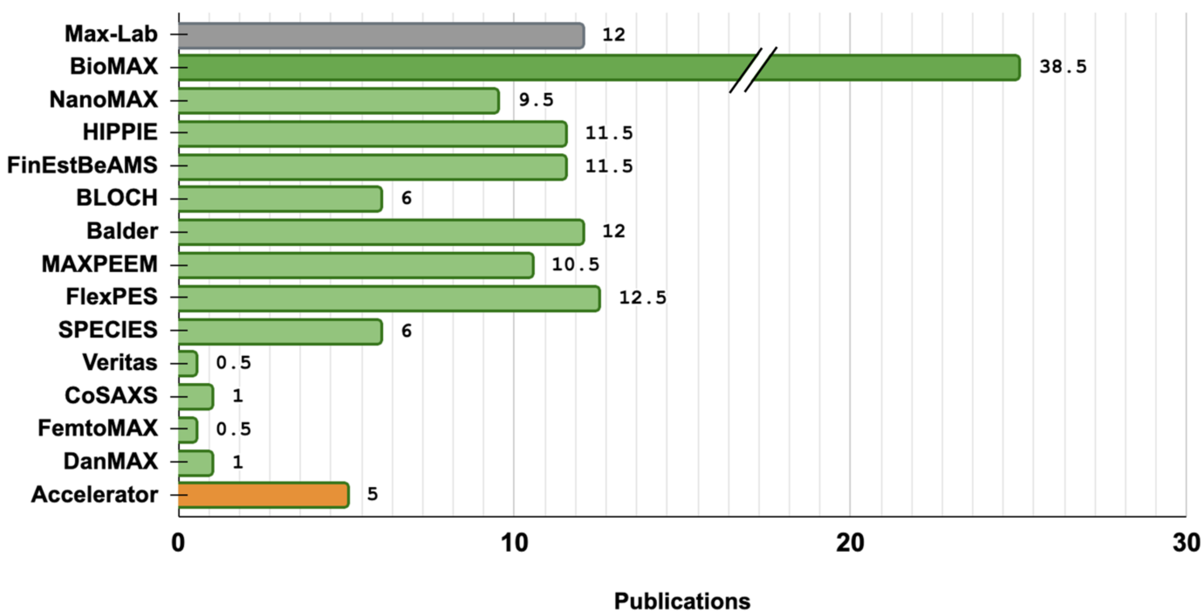

Figure 4: Number of 2021 publications discussing data from MAX-Lab (gray) and the MAX IV beamlines (green). Note that BioMAX is not plotted to scale. Publications related to MAX IV and MAX-Lab measurements are credited with their respective MAX IV beamline. Orange: Number of publications related to our accelerators. Publications based on data measured at more than one instrument are prorated to the number of beamlines involved. Also, beamlines are ordered by introduction to our user programme from top to bottom.

- Beamlines like NanoMAX, HIPPIE, and Balder take full advantage of our small emittance 3GeV ring in the soft and hard X-ray regimes.
- Our most recent beamlines coming online (CoSAXS, FemtoMAX, and DanMAX) are already starting to publish.
- Veritas, our high-resolution X-ray Resonant Inelastic soft X-ray Scattering beamline, suffered from technical difficulties (i.e., internal corrosion of a critical X-ray mirror system) that were addressed in 2021, as described in the beamline development section.
- SoftiMAX is not listed. It should start user operation in 2022.

We also take the opportunity to highlight that in 2021 our staff published various articles documenting and disseminating the technical performance, achievements, and the design of multiple aspects of our beamlines. This was, for example, the case with:

- **FinEstBeAMS** – Chernenko *et al.,* J. Synchrotron Rad. **28**, 1620 (2021)
- **NanoMAX** – Johansson *et al.*, J. Synchrotron Rad. **28**, 1935 (2021)
- **CoSAXS** – Kahnt *et al.*, J. Synchrotron Rad. **28**, 1948 (2021)
- **SPECIES** – Kokkonen *et al.*, J. Synchrotron Rad. **28**, 588 (2021)
- **HIPPIE** - Zhu *et al.,* J. Synchrotron Rad. **28**, 624 (2021)

From the many 2021 publications from our user program, we mention the following scientific highlights:

- Studies on antiferromagnetic spintronics exploiting the beam polarization possibilities at the MAXPEEM beamline (Bommanaboyena *et al.,* Nat. Comm., 2021)
- Studies on biometric wood at NanoMAX (Nissalä *et al.*, Nanomaterials, 2021)
- Studies on hybridization phenomena of the heavy-fermion superconductor $CeIrIn_5$ at Bloch (Mende *et al.,* Adv. Elec. Mat., 2021)
- The demonstration of a successful protein serial crystallography experiment at FemtoMAX (Jensen *et al.,* in J. Synchrotron Rad.,2021) highlights the potential for time-resolved life sciences experiments with our short pulse facility now operating at 10Hz.
- Our online scientific highlights are archived and available online on our website (cf. Figure 5 - Left) at the following link: https://www.maxiv.lu.se/news/category/science-highlights/
- We are also pleased to report on the release of the MAX IV laboratory's "highlights 2020" (cf. Figure 5 - Right) report, which describes our scientific achievements in 2020. It is available on our website at: https://www.maxiv.lu.se/science/reports/.

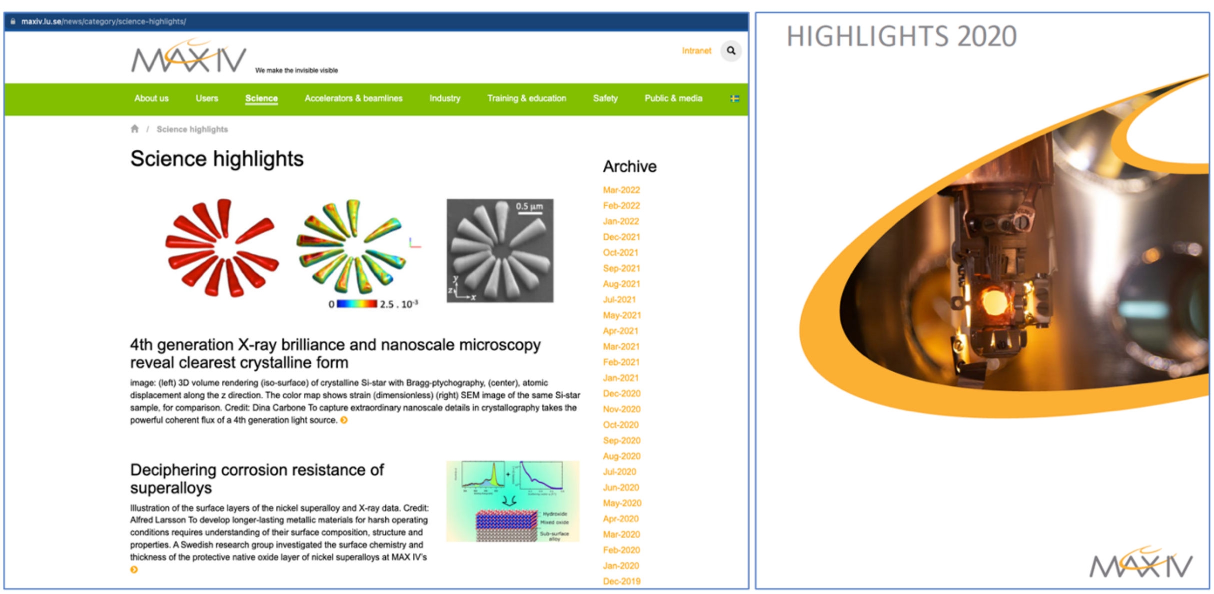

Figure 5: (Left) Screenshot or our webpage providing regular science highlight. (Right) Front page of our "Highlight 2020" publication discussing major science achievements during 2020. It is available on our website at: https://www.maxiv.lu.se/science/reports/

3 User Program

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

- **Fourteen (14)** beamlines were taking X-rays in 2021.
- **DanMAX -** the construction and commissioning of DanMAX progressed well during 2021, and it accepted general users in December 2021.
- **SoftiMAX** – The completion of the construction of the SoftiMAX Scanning Transmission X-ray Microscopy endstation supported commissioning activities throughout 2021. SoftiMAX will accept users in 2022.
- **ForMAX, MicroMAX** – these two beamline construction projects encountered delays because of the Covid-19 pandemic and subsequent chain supply management disruptions. They are expected to accept general users in 2023.
- The details of the extensive capabilities of our beamlines are listed in Appendix 2 but also on our website in our periodical beamline status reports (https://www.maxiv.lu.se/science/reports/)

Impact of the Covid-19 pandemic on our User Program

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

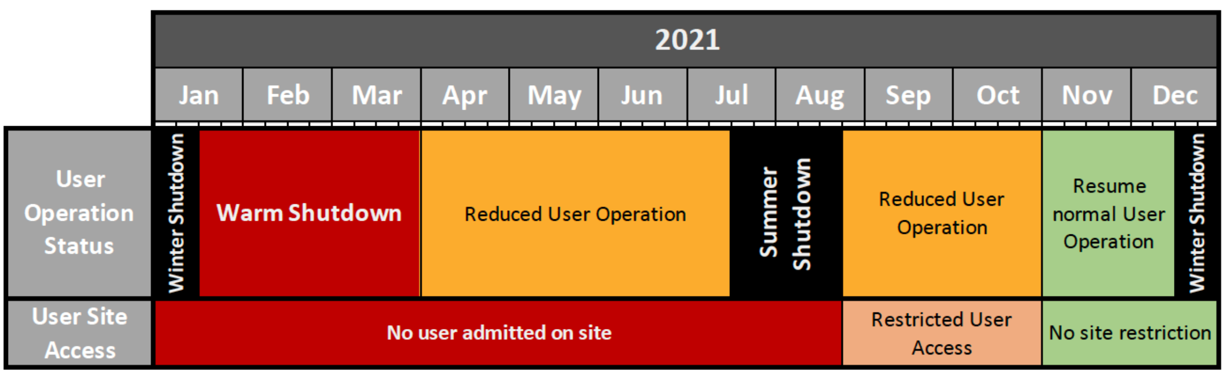

Figure 6:Description of the impact of the Covid-19 pandemic on our 2021 User Program in terms of User Operation Status and User Site Access.

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

This was followed by a phase of reduced operation, during which beamlines gradually resumed user operation one after another. During that time, no user access was permitted. All experiments were performed as mail-in or remotely. BioMAX, our high-throughput beamline dedicated to macromolecular crystallography, is designed to be compatible with mail-in and

remote operation and resumed user operation promptly. The other beamlines evaluated each experiment on a case-by-case basis to assess the possibility or not of performing experiments in any of these two modes of operation: mail-in or remote. This possibility varied greatly from beamline to beamline and with the nature of each experiment.
During the Autumn, access to our facility was gradually restored to full access (normal operation) on November 3rd, 2021. However, international users still encountered travel restrictions, and many experiments had to be cancelled or performed remotely.
In retrospect, 2021 has been very similar to 2020. We observed the cancellation of many user experiments and performed a significant number of experiments without the physical presence of the user group.
For the statistics described in more detail below, we counted each registered user group member for a given experiment as a physical "visit." Each user registered for different experiments is thus accounted for multiple times if listed on different experiments. Still, our User Program Statistics for 2021 presented in this section will preclude any qualitative or quantitative comparison to previously reported data. The number of proposals submitted, accepted, and executed was heavily impacted by cancellation/re-scheduling. Also, the number of our on-site visitors is dramatically decreased.

User Program Statistics

In Table 1 below, we provide statistics related to our User Program for the period running from March 1st, 2021 to February 28th, 2022.
In 2021, MAX IV hosted 1203 user visits. We note that through 2021, site access was precluded most of the year because of the Covid-19 pandemic, as illustrated in Figure 6 (No site access). The distribution per beamline is indicated in Table 1. As mentioned previously, in addition to the usual definition are added those users registered on the proposal for which the experiment was conducted as mail-in or remote. The average gender distribution was 30% women and 70% men.

Balder	88	**DanMAX**	121	**HIPPIE**	96	**SPECIES**	57
BioMAX	271	**FemtoMAX**	29	**MAXPEEM**	90	**STM-lab**	5
BLOCH	82	**FinEstBeAMS**	67	**NanoMAX**	102	**Veritas**	0
CoSAXS	69	**FlexPES**	112	**SoftiMAX**	14		
						Total	**1203**

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

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

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

Table 2: Regional geographical distribution of user visits

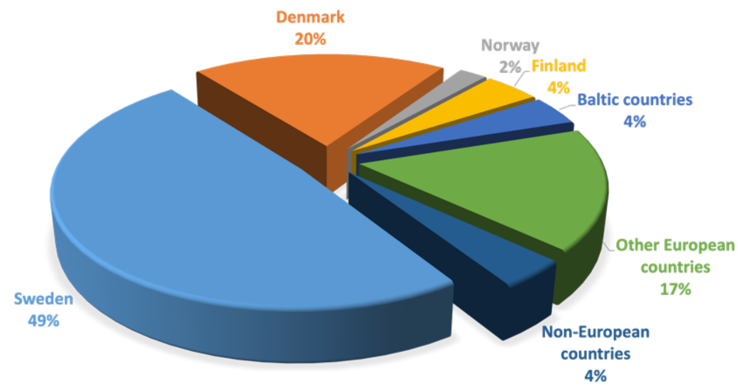

Figure 7: Geographical distribution of the home institution for the recorded user visits for the reporting period.

There were two main proposal calls in 2021.

- The spring call (opened on February 15th; closed on March 16th) accepted proposals that were to be scheduled for the period September 2021 to February 2022. A total of 317 proposals were submitted, and their distribution per beamline is provided in Table 3. The SoftiMAX and Veritas beamlines were not available in this call.
- The autumn call (opened on September 14th; closed on October 5th) accepted proposals to be scheduled for the period March 2022 to August 2022. A total of 309 proposals were submitted, and their distribution per beamline is provided in Table 3**.**
- We note that some beamlines lead in the typical number of proposals per cycle. This is the case with more than 20 proposals per cycle requesting Balder, CoSAXS, NanoMAX, DanMAX, BLOCH FlexPES, HIPPIE, MAXPEEM, and SPECIES. The other beamlines are typically less mature due to a more recent introduction to our user program or different types of proposals, like with BioMAX and BAG proposals.

Figure 8 presents the distribution of submitted and accepted proposals per Program Advisory Committee (PAC) research areas. The MAX IV PAC typically consists of about 55 international scientists. They evaluate proposals based on scientific merit and participate in the beamtime allocation. The current description of the members of our PAC is available at the following link on our website: https://www.maxiv.lu.se/about-us/governance/advisory-bodies/. Before the PAC evaluation, our beamline staff reviews all proposals for technical feasibility. The distribution of our beamlines per research area is provided in Table 3. We note that the largest number of proposal requests by the user community is for spectroscopy, chemistry and soft matter, and nanoscience. Structural biology is not adequately represented in this plot, as this community self-organizes with Beamtime Allocation Group (BAG) proposals.

PAC Research Area	Beamline	Spring Call	Autumn Call
Chemistry & soft matter	Balder	52	51
	CoSAXS	31	24
Structural biology	BioMAX	15	3
Nanoscience	NanoMAX	46	38
Materials science with hard X-ray	DanMAX	17	23
Spectroscopy	FinEstBeAMS	19	19
	BLOCH	22	21
	FlexPES	43	33
	HIPPIE	31	35
	MAXPEEM	18	24
	SoftiMAX	--	13
	SPECIES	20	24
	STM-Lab	2	1
	Veritas	--	4
Ultrafast science	FemtoMAX	5	3
Total		**317**	**309**

Table 3: Distribution of proposals per beamline and call in 2021.

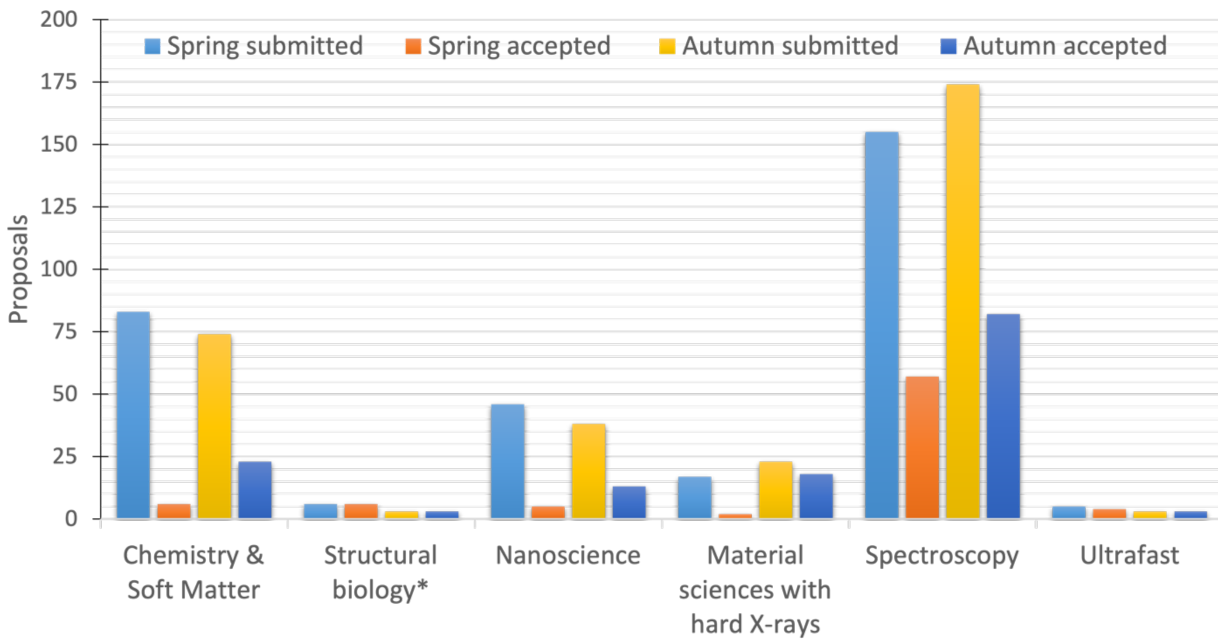

*Figure 8: Submitted and accepted proposals per research area in the 2021 spring and autumn calls. *Structural Biology proposals for the BioMAX beamline include BAG proposals.*

4 Industry engagement

An industry strategy was developed by the Industrial Relations Office (IRO) during the second half of 2020 and approved in March 2021 by the MAX IV board. This strategy focuses on a sector-based initiative approach with four central goals: (i) broaden the industrial user base, (ii) increase the industrial use of MAX IV, (iii) develop MAX IV to support industrial needs, (iv) use a collaborative approach to industry engagement.
This strategy guides industry activities and actions over the coming years and is part of the facility's strategic plan. We have identified ten (10) industry sectors for which the X-ray-based analytical techniques available at MAX IV have a solid potential for impactful industrial research and development. We are actively working on a subset of those sectors with various initiatives to strengthen possibilities to take advantage of the uniqueness of our research infrastructures.
In 2021, the number of industrial users is more than doubled compared to 2020. The amount of proprietary beamtime purchased from MAX IV also nearly doubled. In total, 556 hours of proprietary beamtime were purchased by twenty-seven (27) companies and institutes on seventy (70) occasions during 2021. Table 4 highlights the progression of industrial use of MAX IV since 2018 and provides the breakdown per technique in hours. For each X-ray technique, the respective MAX IV beamlines involved in these beamtimes are listed.
A third of the proprietary beamtime in 2021 was connected to Vinnova pilot projects. A more significant number of companies used MAX IV through the Vinnova pilot project funding, and we also observed an increased number of mediators from academia and institutes.

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

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

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

In January 2021, the IRO team expanded with a full-time member in collaboration with Alfa Laval. This two-year assignment aims to examine how to develop and increase the engagement and commitment to using MAX IV from the R&D activities of the Nordic metal industry. During the first year, the work was focused on understanding the needs of the metal industry and identifying the crucial elements necessary to generate a long-term engagement from both a technical and a business perspective. Also, this was complemented by various forms of workshops and discussions organized with several Swedish companies. Several gaps and areas of improvement have been identified and are used to inform the basis for updating our strategy for future actions.
A new VR-funded project, InfraLife, started at the beginning of 2021. It aims to establish a joint hub between three large-scale research infrastructures: MAX IV, ESS, and SciLifeLab, and to create better access opportunities to the life science industry and health care sector in Sweden. The project adopts a challenge-driven and knowledge exchange approach between the infrastructures. During the spring of 2021, a project addressing anti-microbial resistance resulted in a workshop gathering major stakeholders and during which challenges and opportunities were discussed. The project also focused on mapping ongoing activities, generating outreach materials, and laying the foundation for the activities to be developed in the future.
The Northern Lights on Food (NLF) initiative continued supporting various activities that gather organizations from industry, academia, research institutes, and the industry sector. In June 2021, more than one hundred (100) participants attended the second NLF conference. In November 2021, a second Master Class in food science at synchrotrons focused on imaging techniques and attracted academic and industrial researchers. The Lund Institute of advanced neutron and X-ray science also launched a Northen Light on Food theme, further strengthening the initiative (https://www.linxs.se/northern-lights-on-food)
The MAXESS Industry Arena project continued growing with new partners, and new features are available on the website (https://maxess.se/). Vinnova pilot projects are presented as "easy to read" industry cases on the website as examples of how industry can benefit from large-scale research infrastructures. SmiLe Life Science Incubator joined the project with funding from the EU (regional funds) and Region Skåne to develop a process to connect stepping-stone environments such as SmiLe into the eco-system of service providers around MAX IV and ESS. The project was awarded funding for two years starting from mid-2021.
The collaboration with RISE and Swerim continued through a VR-funded initiative. Partnerships with their staff, MAX IV beamlines, and the MAX IV user community took many forms, including beamline development and commissioning, engagement in the MAX IV strategy process, industry user beamtime, outreach activities, and other joint project activities.

5 Beamline Development

The Covid-19 pandemic undoubtedly severely impacted activities at MAX IV during 2021. This was especially the case for the development of our beamlines. Between January and March 2021, MAX IV was placed in a *warm shutdown*. During that period, only essential personnel was permitted on-site. This period was immediately followed by a *restricted operation phase* that lasted until the end of the summer shutdown, during which access to resources was limited. Prioritizations had to be made, and the focus was set on continuing large installation projects related to our two (2) new beamlines: ForMAX and MicroMAX[1].

The Covid-19 pandemic has resulted in numerous delays in deliveries from many suppliers as a result of restrictions in place but also worldwide disruptions. This affected most projects, especially those involving specialized equipment, semiconductor components and cables. The MicroMAX beamline encountered delays in the delivery of its optical components.

A somewhat unexpected but positive pandemic-related development was that several beamlines introduced innovative ways of conducting remote experiments. For the BioMAX beamline, remote operation was integral to its original plan and was commissioned in late 2020. Therefore, user operation restrictions had a minimal impact on its user program; a hundred and seventy (170) academic and forty-six (46) proprietary four-hour user shifts were performed with no user on site. More importantly, several beamlines, especially those using soft X-rays and for which remote operation was never envisioned, developed ways of supporting this access mode for a subset of user experiments.

At MAX IV, beamline developments are executed as projects and follow two different routes: Central Project Office (CPO) or Beamline Project Advisory Group (BPAG), depending primarily on the scale of the project scope.

The Central Project Office manages large-scale projects consisting of entire beamlines to develop new capabilities or infrastructures for the laboratory. Figure 9 provides the distribution of approved CPO projects per area: common or specific to our beamlines, accelerators and building infrastructure**.** The ForMAX beamline construction projects

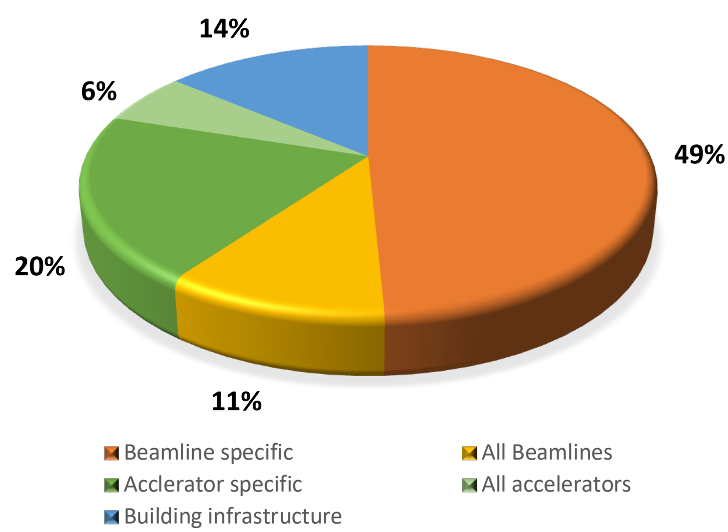

Figure 9: Distribution of approved CPO projects in 2021.

[1] ForMAX is funded by the Knut and Alice Wallenberg Foundation and the Swedish industry via Treesearch – a national platform for research on new materials and specialty chemicals from forest raw materials. The Novo Nordisk Foundation funds MicroMAX.

progressed well in 2021, and its front end is expected to get its first X-rays after the winter shutdown in Feb 2022. The MicroMAX project is also going well and is expected to get the first X-rays later in 2022.

We also note that despite the pandemic, other CPO projects at existing beamlines did progress well, especially for those that had previously completed the installation of components, and therefore principally required software development, and were therefore compatible with remote work. This was, for example, the case for the completion of the SoftiMAX beamline Scanning Transmission X-ray Microscopy (STXM) endstation and at the DanMAX beamline for its diffraction endstation. Both were successfully commissioned by the end of 2021. DanMAX hosted its first general user experiment in December 2021.

At SoftiMAX, work has also started to build a second branch line which will eventually host a Coherent X-ray Diffraction Imaging endstation. DanMAX has procured the main components for its imaging endstation with expected delivery in 2022. DanMAX also secured funding for a third experimental station dedicated to single-crystal X-ray diffraction (SingCrys). The CoSAXS beamline continues to add experimental capabilities, such as time-resolved measurements and a diverse range of sample environments. Following the successful implementation in 2020 of the 10 Hz repetition rate of the linear accelerator, FemtoMAX provided in 2021 short X-ray pulses at that same repetition rate of 10 Hz, a five-fold increase from what was previously available.

Projects of a smaller scale are managed through the Beamline Projects Advisory Group (BPAG) by the Beamline Office (BO) in the Science Division. The year 2021 marked the completion of forty-seven (47) BPAG projects, a number that could have been significantly larger during a typical year, i.e., without the impact of the pandemic. The BPAG projects typically address needs falling into three categories: (i) addition of new capabilities to our beamlines, (ii) improvement to existing beamlines and instrumentation, and (iii) fixes that require immediate attention, as displayed in Figure 10.

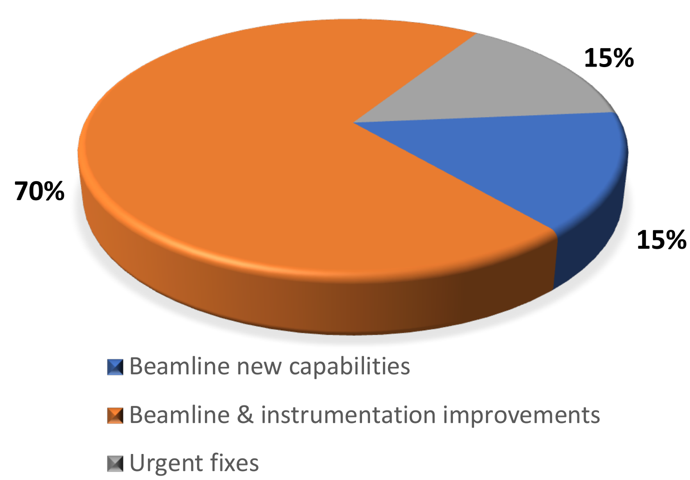

Figure 10: Distribution of approved BPAG projects in 2021.

One of the most visible BPAG projects in 2021 was implementing completely new local cooling water systems on the Veritas and SoftiMAX beamline mirrors. This enabled both instruments to fully accept X-rays, following the corrosion issues previously identified with their internally cooled mirror systems.

New beamlines entering operation in 2021

DanMAX and CoSAXS are now open for general users. At DanMAX, the diffraction station is available for users with a gradual implementation of more capabilities. CoSAXS currently accepts general users for Small Angle X-ray Scattering (SAXS) experiments, while its Wide Angle X-ray Scattering (WAXS) detector is further commissioned. After a six-month delay due to corrosion issues of one of its mirror systems, SoftiMAX started commissioning again and will be open to STXM and Ptychography general users working in the energy range from 275-1600 eV in spring 2022. In the meantime, efforts are directed to extend this X-ray energy range.

New capabilities on operating beamlines in 2021

There have been numerous developments on all MAX IV beamlines during 2021. Below is a non-exhaustive list of some of these achievements:

- **BLOCH -** started commissioning activities on its second branch line dedicated to Spin Angle-Resolved Photo-Emission Spectroscopy (spin-ARPES). Commissioning is expected to continue in 2022, and general users are expected in 2023.
- **HIPPIE** - received funding for a side branch which detailed design was successfully reviewed in June 2021. In addition, the beamline now offers the possibility to combine AP-XPS with FTIR.
- **FinEstBeams** - welcomed its first general users to use its new solid-state endstation.
- **NanoMAX** - tested for the first time their second imaging endstation in December 2021. It is based on Fresnel zone plate optics developed at KTH and will get further commissioned in 2022. It will likely host its first general users by the end of 2022.
- **Veritas** - resumed its commissioning activities following the implementation of a temporary repair of its corroded mirror coupling. It successfully obtained its first high-resolution spectrum from the RIXS spectrometer.

MAX IV also started various initiatives to strengthen and streamline user operation of all beamlines, especially during non-office hours. This is, in particular, the case with the plan to introduce floor coordinators to gradually provide coverage 24/7 during user operation.

6 Accelerator Operations and Development

Accelerator Operations

Accelerator operations in 2021 suffered a significant impact from the “warm shutdown” period implemented as a response to the Covid-19 pandemic in the first few months of the year. Apart from the cancellation of many scheduled beamtimes in the first semester, the pandemic also caused perturbations to accelerator operations in the second semester due to the need to adapt the operations schedule to the delays of various deliveries. This was particularly the case for the late delivery of the insertion devices for the ForMAX and MicroMAX beamlines whose installation was moved from the summer 2021 shutdown to the winter 2021/2022 shutdown.

The resulting scheduled beamline hours for 2021 are 3744, 3888, and 2952 for the 3 GeV ring, 1.5 GeV ring, and Short Pulse Facility (SPF), respectively. These figures fall short of the planned goals for the year by roughly 20% for the storage rings and about 30% for the short pulse facility. Figure 111 shows the evolution of scheduled beamline hours since the start of user operation in 2017.

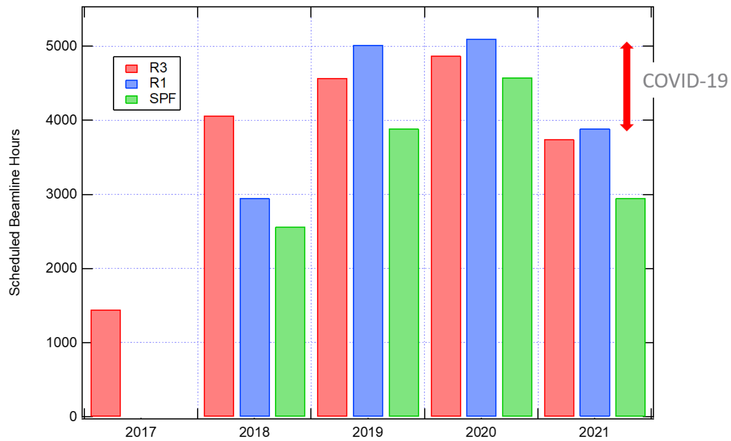

Figure 11: Number of scheduled beamline hours per year since the start of user operations in 2017. By 2020, all accelerators were approaching 5000 hours. The significant reduction in 2021 is a direct result of the COVID-19 pandemic.

The accelerator uptime, which started extremely well with record-high levels for the rings in the first quarter of the year (see, for example, the case of the 1.5 GeV ring in Figure 12), showed a much welcome recovery along autumn after a substantial reduction suffered right before summer. In June, the significant amount of downtime in all accelerators was almost all associated with few (but somewhat long) injector failures, which required interventions to replace faulty klystron tubes. A detailed analysis of the root causes of these failures was performed, which led to setting up a program to address those causes on three distinct levels: (1) to decrease the likelihood of those events through, e.g., preventive replacement of critical components, the introduction of more robust variants of solid-state switches for the klystron modulators, and better diagnostics that can give early indications of upcoming failures; (2) to make interventions on accelerator units faster and less intrusive to operations by providing better tools and training; (3) to work on mechanisms to allow delivering beam to all beamlines in the three accelerators even in the absence of one accelerating unit in the linac, thus making better use of the built-in energy redundancy in the system.

An initial positive impact of those measures was observed in the second half of 2021. The final results for 2021 show that we exceeded the 97% uptime goal for the 1.5 GeV ring (with 97.2% uptime), whereas the 3 GeV ring and the Short Pulse Facility had uptimes very close to their respective goals, namely 96.9% (vs. 97% goal) for the ring and 94.8% (vs. 95% goal) for the SPF.

Another positive result for accelerator operations in 2021 was the significant increase in the Mean Time Between Failures (MTBF) for the two storage rings compared to previous years (Figure 13). This is the result of a systematic effort of identifying and mitigating causes of short

interruptions through measures such as improved automation to reduce the likelihood of human mistakes, review of equipment protection system functional descriptions to avoid overly cautious behaviour that leads to unnecessary beam trips, as well as the implementation of a systematic sequence of dedicated commissioning shifts for newly installed insertion devices. The final MTBF figures for the 3 GeV and 1.5 GeV rings are 79 and 76 hours, respectively, which is significantly higher than the goal for the year (48 hours).
The MTBF for the SPF in 2021 (12 hours) was lower than the yearly goal of 24 hours (cf. Figure 14), and a corresponding MTBF improvement program is planned for 2022. The goal is to address the large number of interruptions that last for a very short time (i.e., a few minutes). Amongst various items in that program, improved automation for the recovery of modulator trips is already implemented.

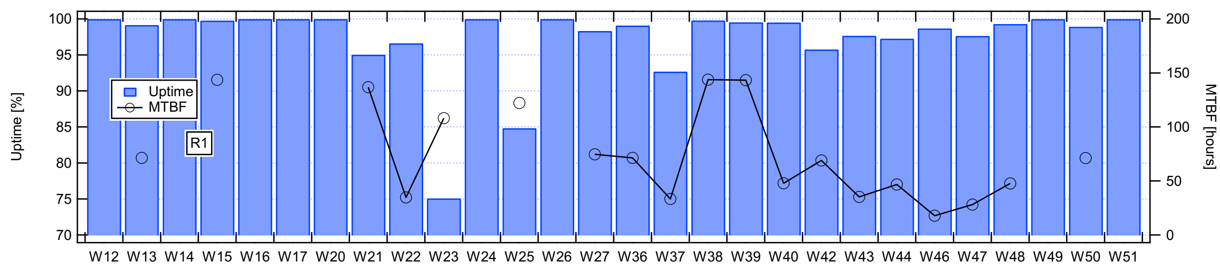

Figure 12: Weekly Uptime and Mean Time Between Failure (MTBF) for the 1.5 GeV ring during 2021. Weeks with 100% uptime have de facto no MTBF.

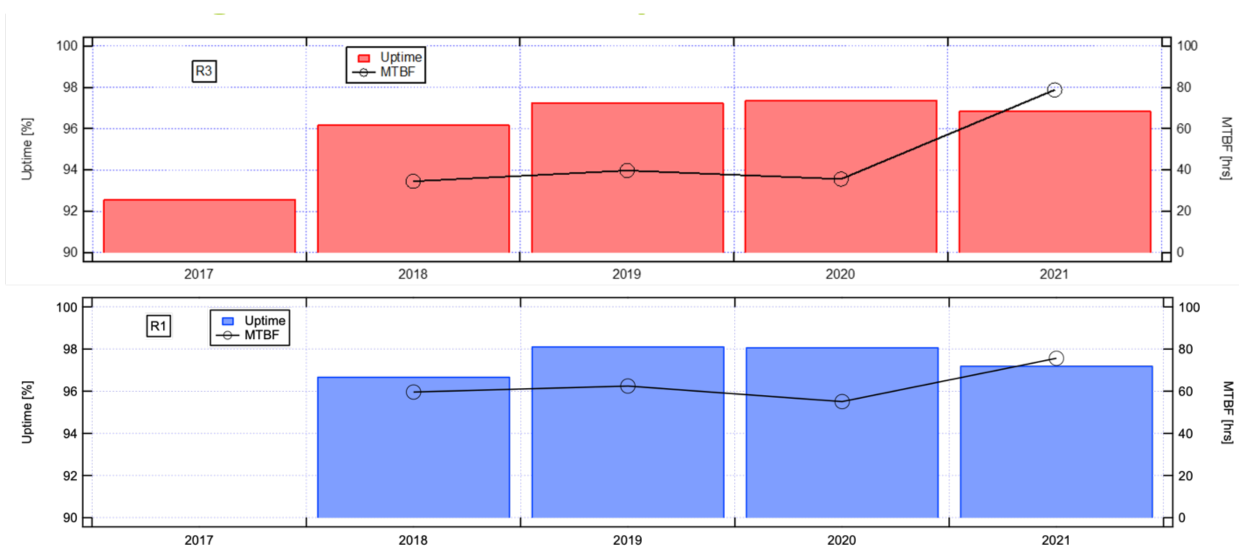

Figure 13: Uptime and Mean Time Between Failures (MTBF) for the 3 GeV (Red) and 1.5 GeV (Blue) storage rings since the start of user operations in 2017. The steady increase of uptime until 2020 is followed by a slight decrease in 2021. The MTBF grows by more than a factor of 2 for the 3 GeV ring and 1.4 for the 1.5 GeV ring from 2020 to 2021. (R1 started operation in 2018)

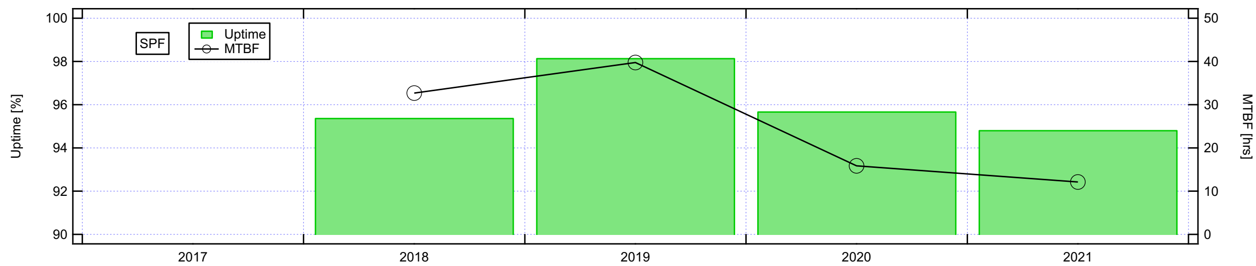

Figure 14: Uptime and MTBF for the Short Pulse Facility. (SPF started operation in 2018)

Accelerator Division Highlights

Completion of the Soft X-ray Laser CDR

The Conceptual Design Report (CDR) for a Soft X-Ray Laser (SXL) driven by the MAX IV 3 GeV linac was completed in late February. The CDR was a joint effort by researchers and engineers at MAX IV Laboratory, Lund University, Lund Laser Centre, Stockholm University, Uppsala University, the Royal Institute of Technology and the Stockholm-Uppsala FEL Centre. It received funding from the Knut and Alice Wallenberg Foundation. The design foresees the production of ultra-short pulses (i.e., down to a few fs) in the 1-5 nm wavelength region with full polarization control and two-pulse/two-color capabilities. It will allow the development of future advanced capabilities such as Echo-Enabled Harmonic Generation, High Brightness SASE, and self-seeding. It will also provide experimental stations with an extensive range of pump lasers from IR to VUV. The SXL Scientific Advisory Committee reviewed the design[2] and congratulated the SXL team for "a very well executed CDR" that "fulfils high international standards." The full CDR can be downloaded from https://www.maxiv.lu.se/soft-x-ray-laser/. The proposed layout of the facility is shown in Figure 15 and the main parameters are summarised in Table 5.

Electron beam energy	3 GeV
Charge per bunch	10 - 100 pC
Wavelength range	1 - 5 nm
Photon pulse duration (FWHM)	0.8 - 26 fs
Photon energy per pulse	0.015 – 1.5 mJ
Maximum repetition rate	100 Hz
Maximum peak brightness	4 x 10^{33} photons s^{-1} mm^{-2} $mrad^{-2}$ per 0.1%BW

Table 5: Main parameters of the Soft X-ray Laser

[2] A SXL CDR SAC meeting was held on February 18-19 and the SXL SAC was composed of Ingolf Lindau (Stanford University, chair), Luc Patthey (PSI), Simone Di Mitri FERMI), Sven Reiche (PSI) and Zhirong Huang (SLAC).

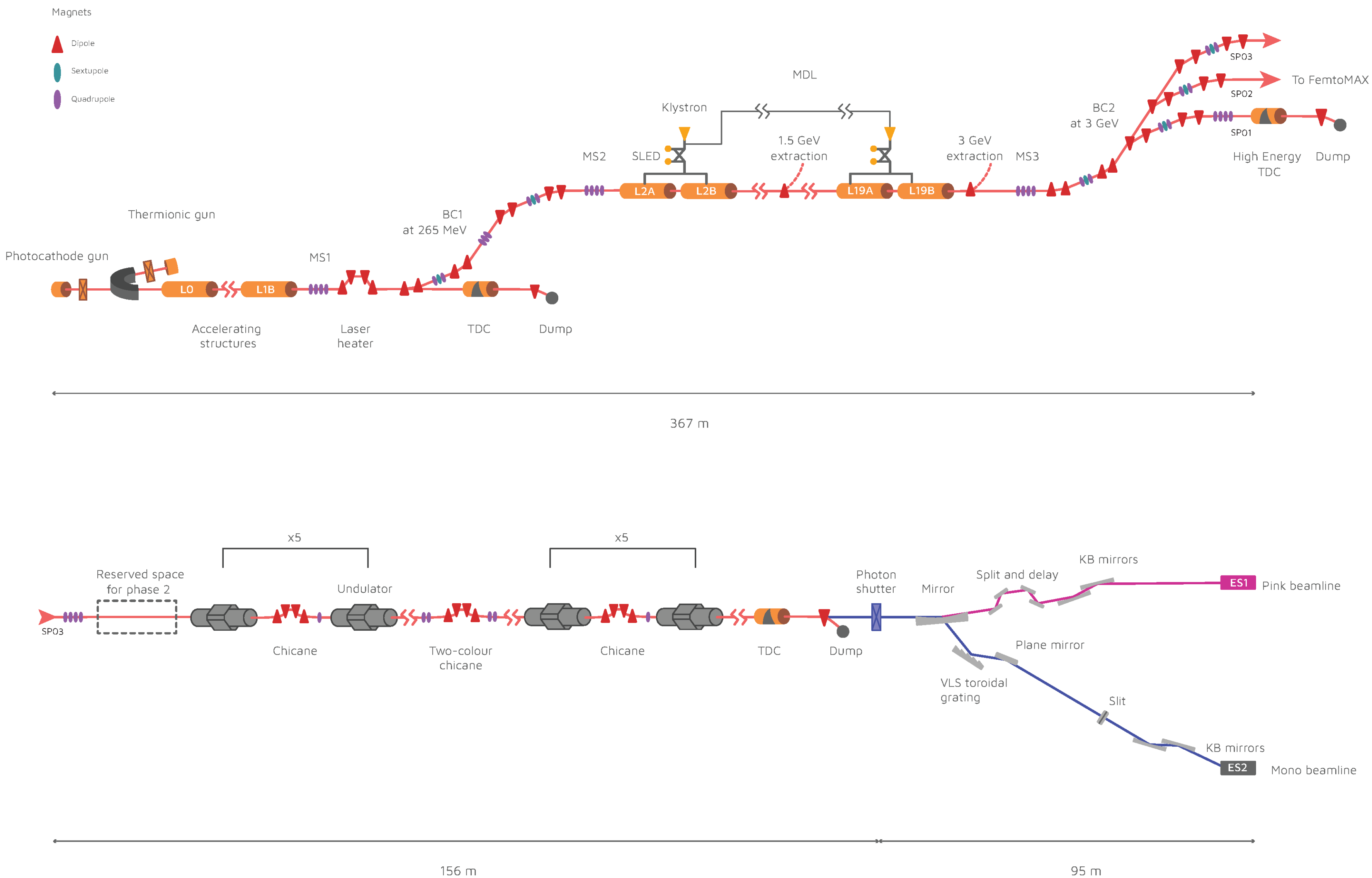

Figure 15: SXL layout. (Top) Existing system with improvements. (Bottom) New systems

Current Increase in the 3 GeV ring.

The stored beam current for routine delivery to the beamlines in the 3 GeV ring was raised from 250 mA to 300 mA in May. This is highlighted in Figure 16, which displays the status of three accelerators on June 20th, 2021. Both rings simultaneously operate in top-up mode and are filled with 300mA and 400 mA for the 3 GeV and the 1.5 GeV rings, respectively.

This was the result of the application of the RCDS (Robust Conjugate Direction Search) algorithm to find optimized settings for the main (100 MHz) and harmonic (300 MHz) rf cavity voltages as well as their temperatures. These procedures allowed the determination of settings for which the currently installed rf plant (i.e., 6 stations with 60 kW each) is capable of providing the necessary power to produce the required accelerating voltages, as well as to fill up the passively operated harmonic cavities and to replenish the energy the beam loses to synchrotron radiation emitted in bending magnets and insertion devices.

Figure 16: Screenshot of the MAX IV Status page on June 30th showing delivery at 300 mA top-up in the 3 GeV ring. It also shows the concurrent delivery of 400mA in top-up for the 1.5 GeV ring and 10 Hz operation of SPF with 70 pC bunch charge.

First beam from the 100 Hz gun

Following the successful implementation, in late 2020, of operation of the linear accelerator at 10 Hz for delivery to the Short Pulse Facility and injection into the storage rings, focus now shifts to further increases towards the final goal of 100 Hz repetition rate. A significant milestone in that project was achieved on October 21st, when the first electrons from a new radiofrequency photo-cathode gun were observed (6) at the MAX IV Gun Test Facility (GTF). The new gun, shown in Figure 17, features improved coupling slots to utilize the SLED pulse better, leading to a reduced probability of sparks around the coupling holes, improved curvature of irises inside the gun to decrease the maximum field amplitude on the surface, and improved design of the cooling circuits.

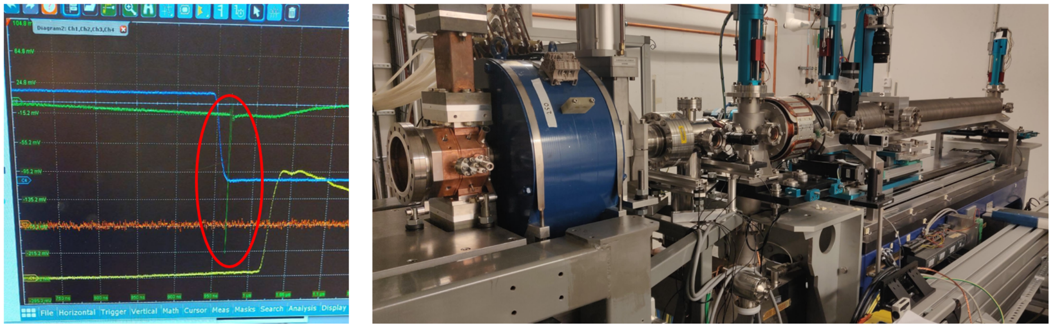

Figure 17: (Left) First electrons extracted from the new 100 Hz gun at the Gun Test Facility. (Right) The gun as installed at the Gun Test Facility (GTF).

Beam size reduction for the FemtoMAX beamline

As a result of several improvements to the linear accelerator, including better diagnostics and more flexible control of the electron beam optics, a significant reduction of the electron beam emittance and electron beam size at the FemtoMAX undulators was achieved, as shown in Figure 18.

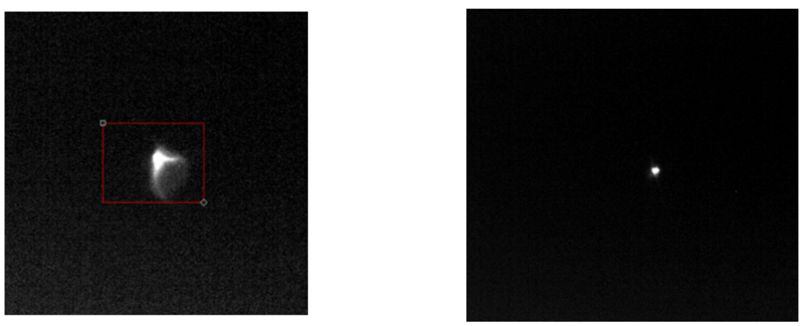

Figure 18: Improvement in electron beam size at the FemtoMAX undulators obtained in 2021 as a result of several improvements to the linear accelerator. (Left) The electron beam size is roughly 230x230 μm2 (FWHM). (Right) After correction, the electron beam size is 150 μm in both the vertical and horizontal directions.

First results from a Beam Arrival Monitor (BAM)

Pulse-to-pulse stability of the electron bunches delivered by the linear accelerator is a critical performance parameter for the experiments carried out with the X-ray pulses produced at the Short Pulse Facility. Particularly important for the efficient use of very short X-ray pulses (nominally down to 100 fs delivered to the FemtoMAX beamline) is the repeatability of electron beam arrival time. A prototype Beam Arrival Monitor (BAM) based on a resonating cavity pick-up was installed in late 2020 at the MAX IV linac to detect the arrival time of the bunches having the linear accelerator master 3 GHz oscillator drive signal as a reference. First results emerged in autumn 2021 and showed a measured resolution and arrival time jitter better than 50 fs rms, as displayed in Figure 19.

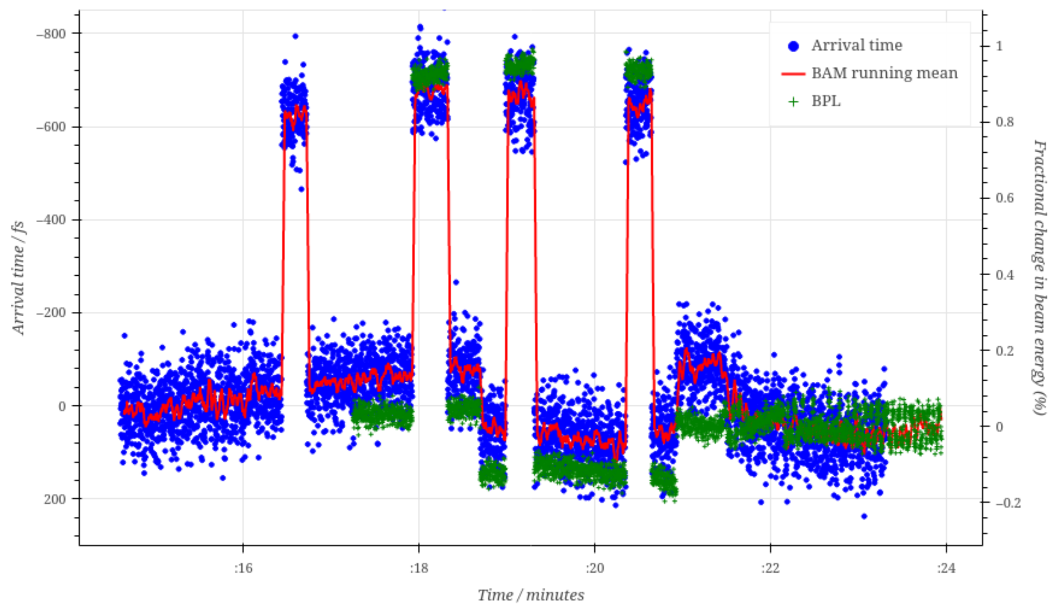

Figure 19: Beam arrival time and beam energy measurements. Blue is the arrival time, whereas red is the relative energy deviation as determined by the change in beam position at a dispersive point of the lattice. The four large steps at around 17, 18, 19, and 21 m minutes were generated on purpose by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

Project "B.O.R.I.S"

Blue-lining is a time-consuming process required to correctly define positions on the floor for supports and components for accelerators and beamlines. At MAX IV, this is typically carried out by engineers in the Survey, Alignment, and Mechanical Stability (SAM) Team, in the Engineering group. SAM is developing a high-precision self-positioning blue-lining robot that would significantly improve the existing method. The goal of the Blue-lining Optimal Robotic Imprinting System ("B.O.R.I.S") project is to build the robot through a collaboration between MAX IV and the Engineering faculty at Lund University (LTH). The project concept was presented at the EU Robotics Week 2020. The first prototype results were the topic of a Master thesis presented by Lisa Klinghav (Figure 20) at LTH in March 2021 under the co-supervision of Alina Andersson (Figure 20), a research engineer in the MAX IV SAM team. In November 2021, the project received an additional boost through an external funding grant awarded by The Royal Physiographic Society of Lund. Moreover, this project collaborates with the SBUF development project by Peab, Cognibotics AB, and LTH (Buster - construction robot dog based on Spot from Boston Dynamics).

Figure 20: Lisa Klinghav (left) and Alina Andersson (right) celebrating the robot's first blue-lining in the lab (Credit: Lisa Klinghav)

7 Collaborations and Partnerships

Project Applications

In 2021, MAX IV was involved in forty-eight (48) individual grant applications to national and international funding organizations. In about 40% of the cases, the main applicant of the project was a MAX IV staff (with or without project partners). The remaining 60% of the applications were led by external collaborators from various domestic and international institutions, as displayed in Figure 21. This highlights the strength of the proactive approach of MAX IV researchers in applying for funding and shows that strong links exist with collaborators from academia and industry.

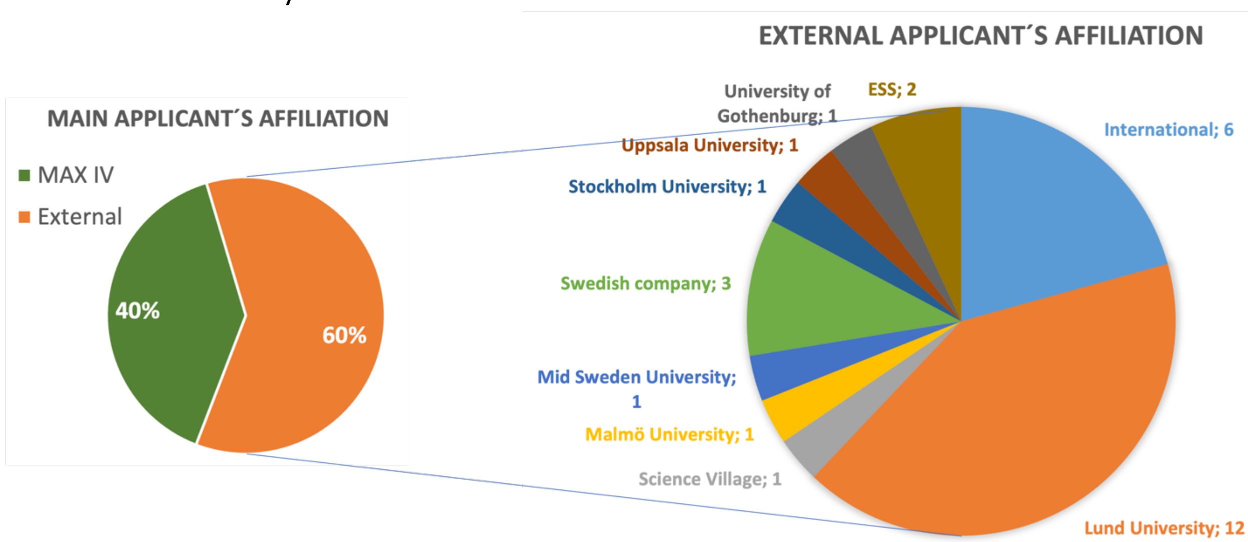

Figure 21: (Left) Graphical distribution of the affiliation of the main applicant of each project application. (Right) Number of project applications per main applicant affiliation involving MAX IV as a partner.

The forty-eight (48) project applications were submitted to eighteen (18) different funding agencies, sixteen (16) of which are from Sweden, as displayed in Figure 22. We also note the following:

- Twenty (20) applications were approved, corresponding to a success rate of 41%.
- Eight (8) out of the fourteen (14) applications submitted to the Swedish Research Council (VR) were for the Röntgen-Ångström Cluster Call. In contrast, four (4) of them were submitted to the call for investment in existing research infrastructure.
- Of the four (4) applications sent to Vinnova, two (2) were submitted to the call for the Industrial utilization of technologies based on neutron and synchrotron light at large-scale research infrastructure.
- The MAX IV Industrial Relations Office has received a 1.4 MSEK grant from Tillväxtverket in the context of REACT Call to finance the MAXESS Industry Arena project. This is a starting point for industrial researchers who need to know how synchrotron- and neutron-based techniques and methods can support their research and development.

- Three (3) of the six (6) applications sent to European Commission Programs were submitted to Horizon 2020 Calls.

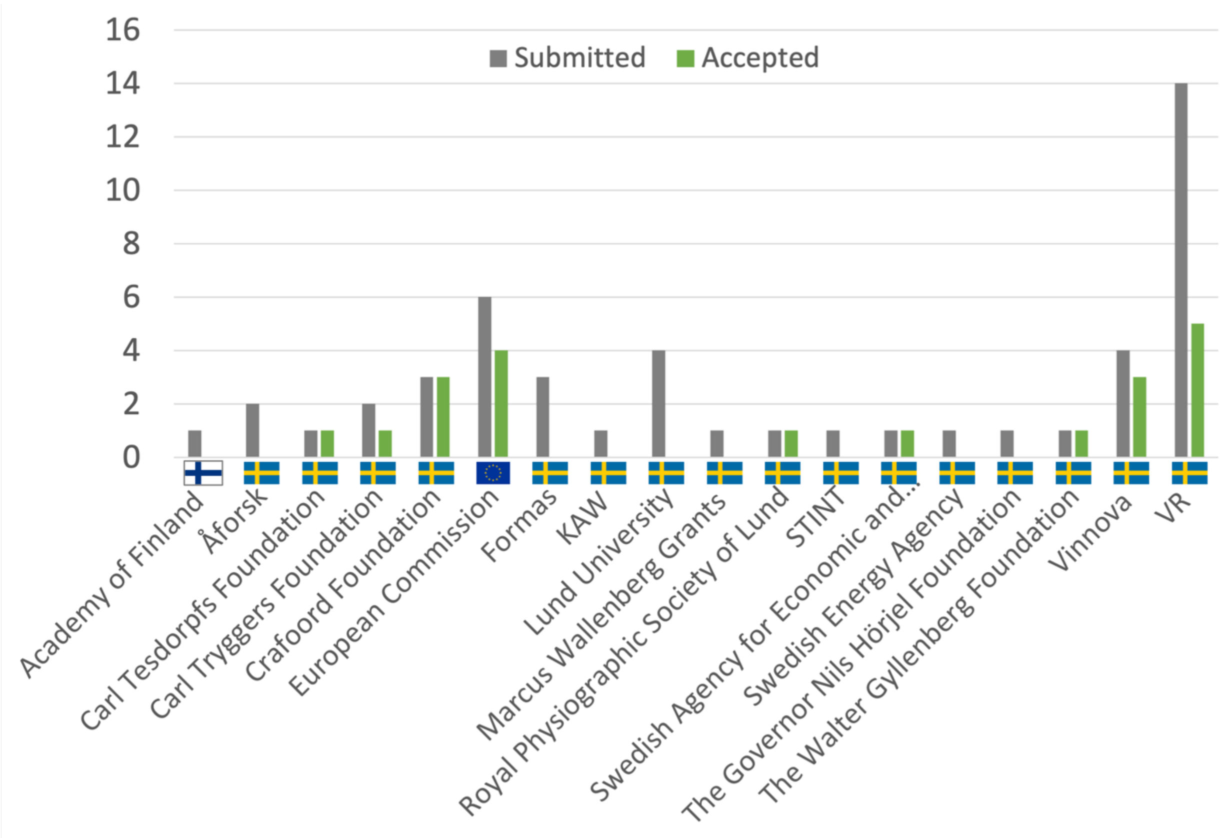

Figure 22: Number of applications submitted and approved per funding agencies in 2021 (known as of Feb 2022). Submitted applications without currently known outcomes are not shown. Funders are listed alphabetically.

Funded External Research Projects

The following paragraphs outline a summary of (A) the currently ongoing projects that started before 2021 and those (B) that started in 2021 (i.e., approved towards the end of 2020 and during 2021).

A. Ongoing Projects

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

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

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

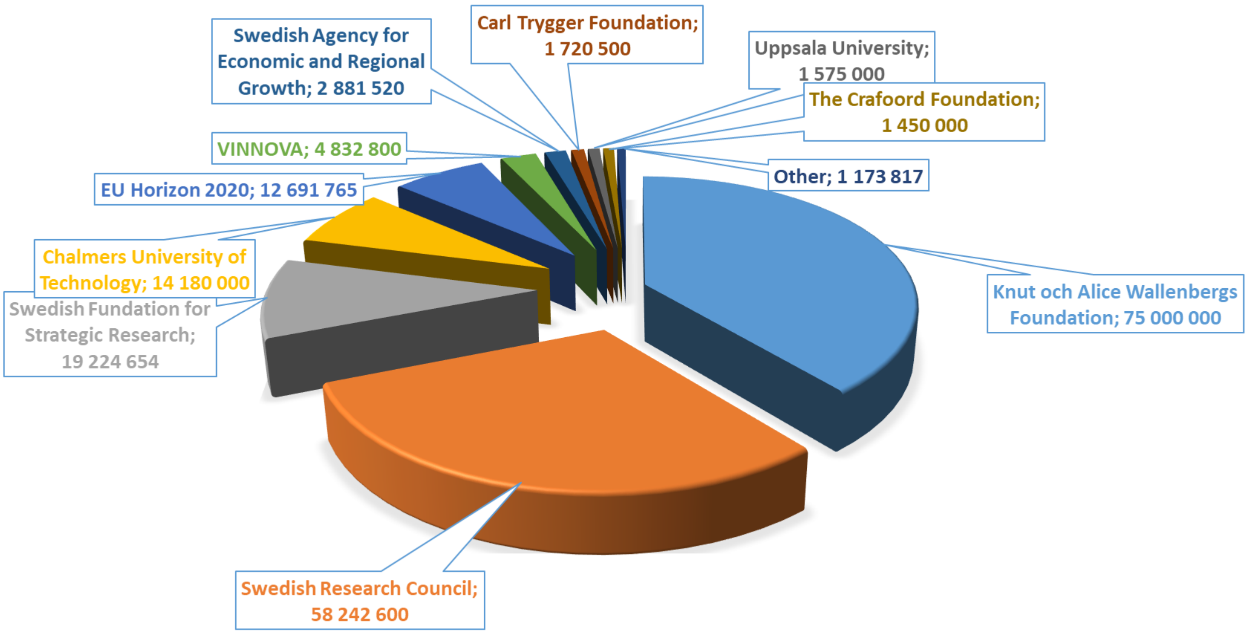

Figure 15: Contract amount in SEK per Funding Agency in 2021 for a total amount of 192 972 656 SEK. The indicated values do not include projects that ended during 2021. The grant values relate only to research projects and do not include funding for beamline construction projects.

B. New projects in 2021

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

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

- **Collective dynamics with coherent X-rays**
  This funded project was directed towards developing the use of X-ray coherence by procuring a state-of-the-art detector for fast time-resolved X-ray photon correlation spectroscopy (XPCS) in collaboration with the user community.
- **TRISS – Trapped Ion Spectrometer Setup**
  This funded project aimed at developing a set of internationally unique and competitive instrumentation that facilitates trapped ion x-ray spectroscopy. This is relevant for many scientific areas: molecular physics, biomolecular research, clusters/super-atoms, energy materials, atmospheric chemistry, astrophysics, astrochemistry, astrobiology, and surface physics.
- **Upgrade of the AC-SPELEEM microscope with a new energy analyzer and detector of electrons**

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

Ongoing collaborations

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

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

8 Communication and Outreach

The communication effort at MAX IV is twofold: (i) the internal communication aims at promoting building blocks of a communicative organization such as dialogue and transparency, (ii) the external communication has target groups such as existing and prospective users, stakeholders, education organizations, and the public.

To streamline internal communication, a monthly internal newsletter was initiated in 2021. It consists of updates from all MAX IV divisions. An internal communications strategy with short- and long-term goals was drafted for further internal discussion.

A significant part of the external communication in 2021 was directed to support the MAX IV Strategy and Roadmap with adapted web content (cf. https://www.maxiv.lu.se/about-us/strategy/), workshops, and newsletters. Sixteen (16) workshops (cf. https://www.maxiv.lu.se/about-us/strategy/workshops/) were organized in the second half of 2021 to connect the user community to the Strategy and Roadmap and gather community input. The Covid-19 pandemic impacted access to MAX IV and many of our outreach efforts. Our yearly Open Days public event and our summer school were cancelled, in addition to several study visits. The MAX IV Annual User Meeting was the largest external event organized in 2021. It consisted of a hybrid meeting with around four hundred (400) attendees from academia and industry, half of whom attended remotely. Many of the sessions were live-streamed to be accessible for those who could not travel and attend the venue because of pandemic-related travel restrictions. The sessions covered beamline updates, user science, and the talks by the student and PhD awardees. Several sessions were also dedicated to the MAX IV strategy and roadmap process. Details of the programs can be found at https://www.maxiv.lu.se/users/user-meetings/user-meeting-program-2021/.

We also drive the editorial process that leads to the publication of the laboratory's "Highlights 2020" document that describes the scientific achievements of the laboratory. It can be consulted at the following link: https://www.maxiv.lu.se/science/reports/.

Other parts of our external communication and outreach programs are the external newsletter, study visits, workshops, and our presence on social media. In 2021, we continued to develop our website http://www.maxiv.se and produced an updated version to comply with Swedish accessibility regulations. It will be launched in 2022. We note a steady increase in the number of visitors to our website, exceeding a hundred thousand (100000) unique visitors, in 2021, as displayed in Figure 24. We also notice a steady increase in our digital media footprint, as shown in Figure 25, with a growing number of followers on LinkedIn, Twitter, Facebook, and Instagram.

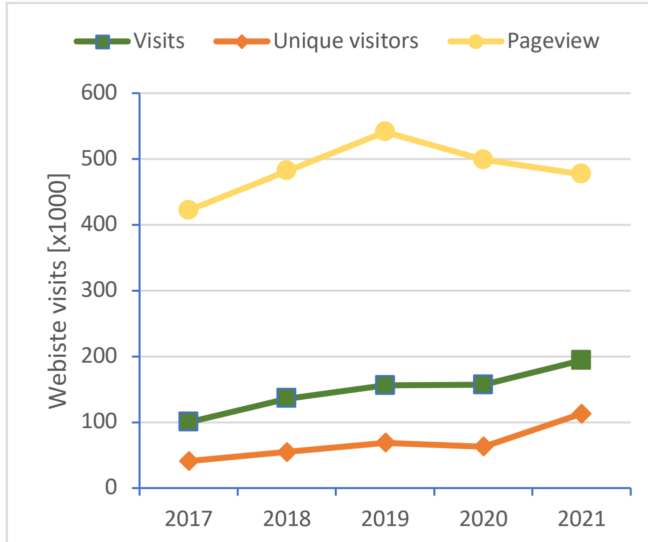

Figure 16: Statistics of access to the MAX IV website (http://www.maxiv.se) in thousands of visits, unique visitors, and page views.

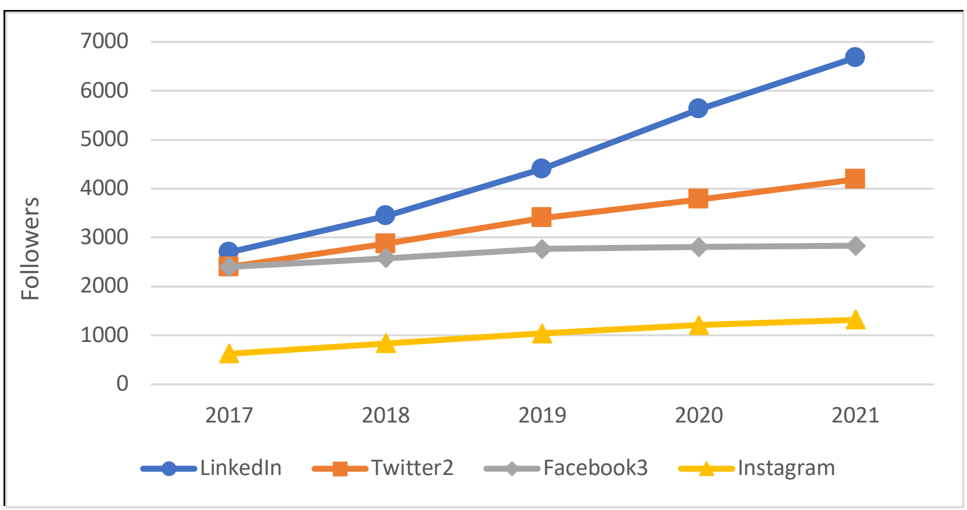

Figure 17: Statistics of MAX IV social media followers for LinkedIn, Twitter, Facebook, and Instagram

Our collaboration with the European Spallation Source (ESS) on outreach was strengthened, and a workshop was held at the local school Fäladsgården. Architects from FOJAB were engaged to lead the pupils in proposing components for an ESS/MAX IV activity space and playground in the Brunnshög area.

9 ORGANISATION AND STAFFING

The details of the MAX IV organization by year-end 2021 are shown in Figure 26. Details on the MAX IV governance, including the descriptions of the MAX IV board and the various Machine, Scientific, and Program Advisory Committees (MAC, SAC, PAC), are provided on our website at the following link https://www.maxiv.lu.se/about-us/governance/.

At the end of 2021, MAX IV consisted of 279.5 Full-Time Employees (FTE), as displayed in Figure 27. MAX IV continues to steadily grow as an organization while constructing, commissioning, and operating an increasing number of beamlines. Most of our open positions are advertised internationally to seek the strongest possible candidates, thus resulting in about half of our employees being from countries other than Sweden.

The search for a permanent Physical Sciences Director initiated in autumn 2020 concluded. Following the recommendation from the MAX IV Director to the MAX IV Board, the recruitment of a Physical Sciences Director was completed in 2021. Dr. Aymeric Robert started full-time employment on October 4, 2021, as indicated in our org chart presented in Figure 26.

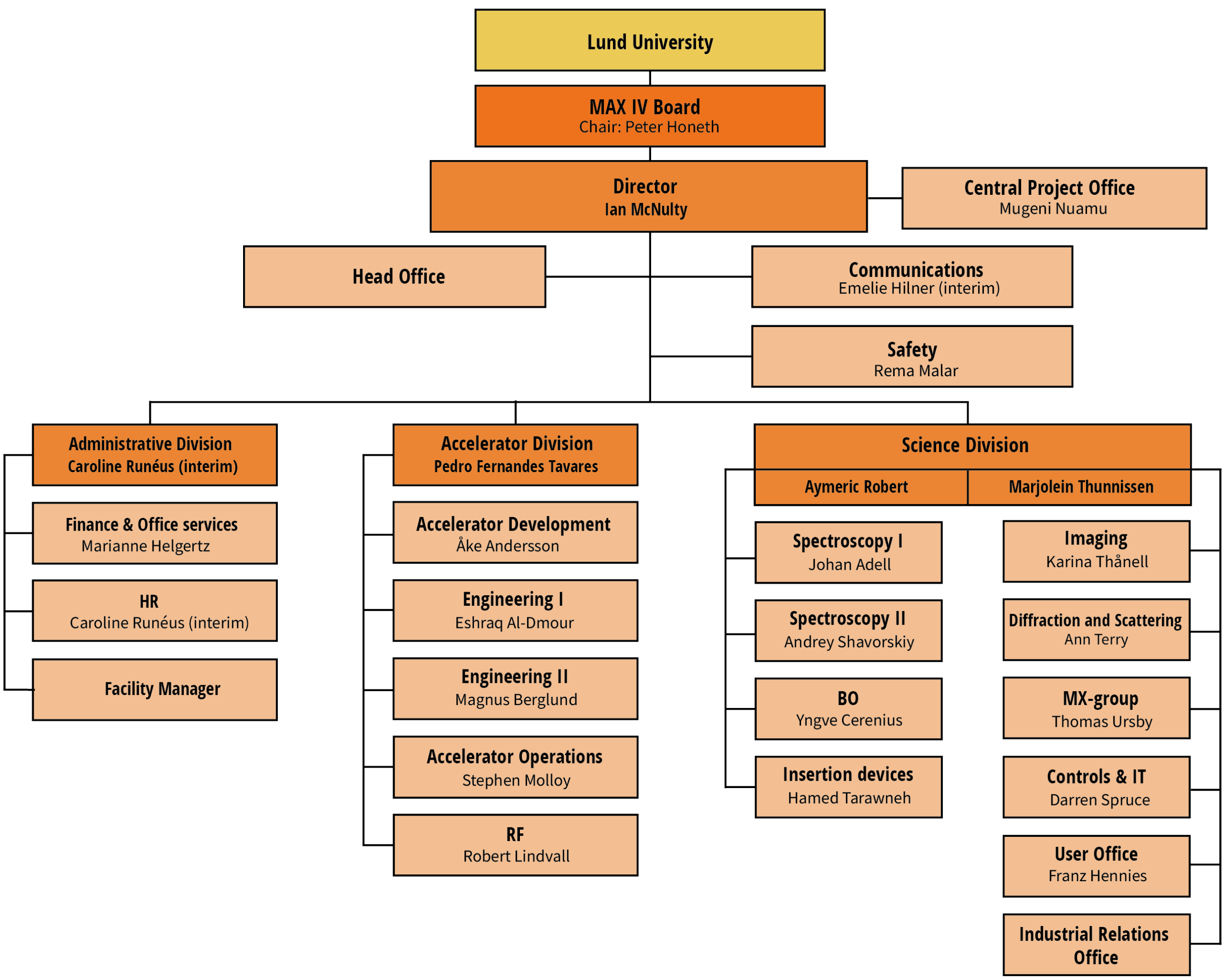

Figure 18: MAX IV Laboratory organisation chart as of December 2021 that details the Administrative, Accelerator, and Science divisions and their groups and central functions such as Communication, Safety, and the Central Project Office.

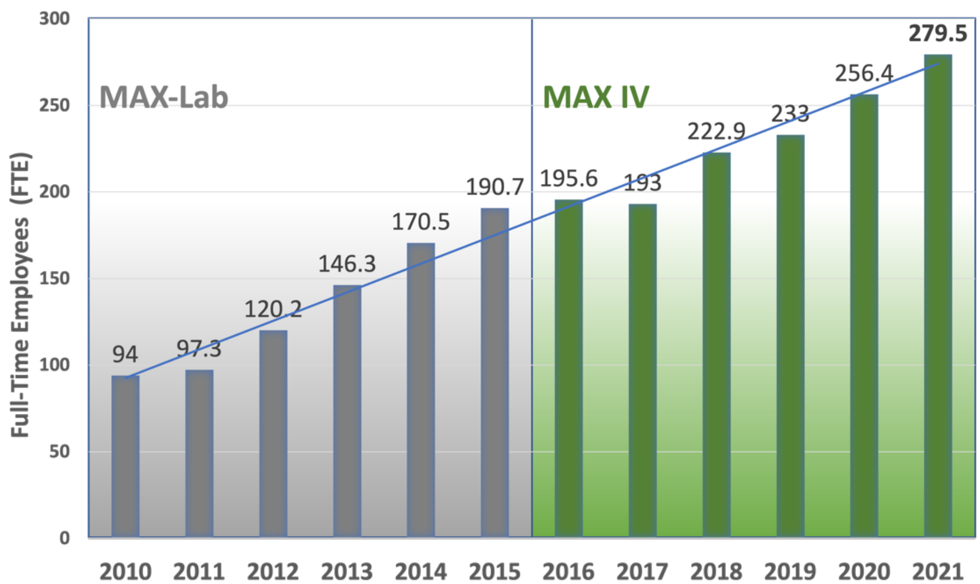

Figure 19: Number of Full-Time Employees (FTE) since 2010. MAX IV Laboratory opened its door to staff in January 2016. Before this date, the laboratory was called MAX Lab.

The MAX IV Board initiated a review of the organization in 2021 to analyse if it is optimally adapted to its current and future needs. This was also driven by identifying how to support the core business of the laboratory better. This review involved many discussions with the employees. It led to the recommendation to establish a Technical Division consisting of pooled resources within engineering, controls, and IT services. This follows a preceding recommendation in the same direction by a review committee established by Vetenskapsrådet, aka the Swedish Research Council. The MAX IV Board decided at the December 2021 meeting to move ahead with forming a new Technical Division. The recruitment of a Technical Division Director and the division's formation is expected to occur in 2022. During the same organizational review, emphasis was also placed on analysing how some functions at the core of organizational support could optimally support the laboratory's mission. This has not yet led to a recommendation for an organizational change.

In April 2021, an organisational and social work environment survey was conducted. Compared with a similar survey conducted two years earlier, the results showed an overall improvement. However, the study also indicates clear areas for improvement: leadership, internal communication, and work environment. The survey also highlighted a strained situation for the middle management in the organization. This has been further exacerbated by the Covid-19 pandemic, as remote work for most staff created an extra workload on managers. An action plan to improve these areas is in progress.

During the Spring and Autumn of 2021, a leadership development program was conducted for ten newly employed managers and 20 team leaders. The purpose of this training was to better understand the role and responsibilities of staff in a leadership position.

10 Financial report

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

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

Comments on the outcome of the 2021 MAX IV Operating Budget

Details regarding funding, costs and results are provided in Appendix 4. MAX IV delivered a result of -20.6 MSEK and hence a corresponding decrease in agency capital. The outgoing agency capital in 2020 was 35.1 MSEK.

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

Comments on Funding

We provide below more information for some of the deviations of funding in 2021:

A. A new agreement was signed with the University of Tartu regarding the Estonian contribution to the operating budget. This results in a net addition of +0.6 MSEK.
B. The total income from proprietary beamtime sales resulted in 4.1 MSEK instead of the budgeted 2 MSEK.
C. Other incomes - MAX IV accounts for revenue from the sale of recycled heat, hosted conferences, etc.; some of which was overestimated (-1.6 MSEK)

Comments on Costs

Throughout 2021, we observed that most groups spent less than budgeted due to the many impacts of the Covid-19 pandemic. Attendance at domestic and international technical and scientific conferences, business travels, and other similar activities was cancelled. In addition, many meetings (i.e., MAX IV Board, Scientific and Machine Advisory Committee and Programme Advisory Committee) were held digitally or in a hybrid form that directly reduced the cost of such activities.

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

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

A. The observed decrease in rent originated from a lower STIBOR index than the budget.
B. Despite the prevailing high electricity prices, the costs did not deviate from the budget. The variable cost of electricity was partially fixed (70%) throughout 2021 according to the terms of agreement with Entelios, a professional trading company in the financial electricity market.
C. Staff cost (excluding staff in the following groups: Accelerator, Life and Physical Sciences, IT & Controls, and Engineering I&II). We filled positions at a faster rate than budgeted.
D. The observed increase is attributed to larger consulting costs than expected.
E. Staff costs for the Life Sciences beamlines in the Science Division are 30.3 MSEK.
F. Staff costs for the Physical Sciences beamlines in the Science Division are 38.5 MSEK.
G. Staff costs for the IT & Controls groups are 33.5 MSEK
H. The contribution to LUNARC, the center for scientific and technical computing at Lund University, has been less than budgeted.
I. Staff costs for the Engineering I & II groups are 17.5 MSEK
J. Delays in investments for accelerator upkeep and developments affect depreciation.
K. In-kind contributions from 14 Swedish universities were more significant than budgeted.
L. The use of management contingency was less than budgeted.
M. Upkeep of planned allocation of VR grants: 80.5 MSEK
N. Undepreciated funds from VR grants: 125 MSEK
O. Agency capital is 31.5 MSEK

11 Financial outlook 2022

The operating budget for 2022 was approved by the MAX IV Board in December 2021. The total funding for 2022 is budgeted for 491,6 MSEK. The Swedish Research Council contributes with 365 MSEK (74%). The remaining funds are provided by Vinnova, Formas, the 14 Swedish universities, additional contributions from Lund University, contributions from Finland and Estonia to the operating budget. As in previous years, we expect extra income from selling proprietary beamtime, recycled heat, etc.
We note that:

- The warranty period in the lease for the building expired in 2021. This implies that MAX IV is now responsible for all costs related to the building infrastructure. A facility manager was recruited to actively manage tasks related to this end. To support the scope of work of this new function, a property management system (AFF) was deployed and will allow better management of maintenance needs for our building infrastructure. The complexity of our facility and the need for operational reliability set high demands on partnering with an external supplier with extensive experience in technically advanced operations.

- In October 2021, the international maintenance firm, Caverion, was contracted to support us with this task. Caverion's assignment includes technical management, supervision, and maintenance of technical infrastructure installations such as ventilation, cooling, heating, control and regulation, electricity, fire and security, passage and locking systems, emergency preparedness, customer service, and fault reporting. Via Caverion Remote, the building infrastructure is monitored 24/7.
- Rent cost is assumed to remain stable through 2022 as the interest rate remains nearly zero (0% STIBOR 3M). As the staff increases, the estimated cost corresponding to office space is included in the budget.
- The variable cost of electricity is partially fixed (70%) throughout 2022. As the market uncertainties are significant, MAX IV has budgeted for 5% more power consumption and 25% higher electricity prices than in 2021.
- On the staffing side, MAX IV is planning to continue to invest in its level and quality of user support by completing the hire and deployment of floor coordinators on/call technical services.
- Following the recommendation from the MAX IV Board and the Swedish Research Council, MAX IV is moving forward with recruiting a director that would lead a Technical Division. This newly formed division would consist of most existing engineering and controls & IT groups and would centrally manage and provide pooled resources to the whole laboratory.
- An annual program for in-house application of funding will be introduced in 2022 to replace or acquire instrumentation and development projects connected to maintaining the performance of our beamline and keeping them competitive.

Appendix 1 List of Abbreviations

APXPS	ambient pressure x-ray photoemission spectroscopy
ARPES	angle resolved photoelectron spectroscopy
BAG	block allocation group
BAM	beam arrival monitor
CPO	Central Project Office
CTH	Chalmers University of Technology
DDR	detailed design report
ESS	European Spallation Source
E-mynd	Swedish Energy Agency
EXAFS	extended x-ray absorption fine structure
FEL	free electron laser
GU	Gothenburg University
IRO	Industrial Relations Office
KAW	Knut and Alice Wallenberg Foundation
KI	Karolinska Institutet
KITS	Controls and IT group
KTH	KTH Royal Institute of Technology, Stockholm
KU	Karlstad University
linac	linear accelerator
LiU	Linköping University
LnU	Linnæus University
LTU	Luleå University of Technology
LU	Lund University
MU	Malmö University
PAC	Programme Allocation Committee
RF	radio frequency
RIXS	resonant inelastic X-ray scattering
SAXS	small angle x-ray scattering
SLU	Swedish University of Agricultural Sciences
SPF	Short Pulse Facility
SU	Stockholm University
SXL	soft x-ray laser
UmU	Umeå University
UU	Uppsala University
Vinnova	Swedish Governmental Agency for Innovation Systems
VR	Swedish Research Council
WAXS	wide angle x-ray scattering
XANES	X-ray absorption near edge structure
XMCD	X-ray magnetic circular dichroism
XPCS	X-ray photon correlation spectroscopy

Appendix 2. Beamline Capabilities available to users

Beamline	Techniques	Energy	Capabilities available to users
Balder	XANES, EXAFS	2.4-40 keV	XANES and EXAFS in transmission, continuous scanning to 30 s/EXAFS XANES and EXAFS in fluorescence with 7 element SDD, continuous scanning to 30 s/EXAFS
BioMAX	MX at fixed energy, MAD, SAD	6-24 keV	Remote data collection Automated sample mounting and dismounting from UniPucks, 29 puck positions in dewar Beam focus of 20x5 µm, 50x50 µm or 100x100 µm and defining aperture of 5, 10, 20, 50 and 100 µm Element identification by X-ray fluorescence Fragment-based drug screening Serial crystallography using HVE-injector (high viscosity extrusion injector), fixed target scan using MD3
Bloch	ARPES	15-200 eV (10-1000 eV with less flux /resolution)	High-resolution ARPES with deflection based analyser or 6-axis manipulator Linear vertical or horizontal polarised light, with energy range 10-1000 eV (peak flux and resolution 15-200 eV) Online STM, 50K – 300K In expert commissioning: Spin-resolved ARPES with a 3D-VLEED detector
CoSAXS	SAXS/WAXS	12.4 keV (fixed energy)	SAXS, q-range 1×10-3 to 0.7 Å-1 Laser triggered, temperature jump time-resolved SAXS (2 ms time-resolution), q-range 1 x 10-3 to 0.5 Å-1 and ca. 1.5 to 2.3 Å-1 Solution and bio-SAXS, with pipetting autoloader from 96 well plates, flow-through quartz capillary, in-line HPLC Multiple capillary, multiple position solid sample holders, with thermostatic water bath; Linkam heating stage with liquid nitrogen cooling pump. SAXS/WAXS, at 12.4 keV, q-range 1 x 10^{-3} to 2.0 Å^{-1} Microfluidic sample environment
			Veritas B (open port)

Beamline	Techniques	Energy	Capabilities available to users
DanMAX	PXRD	15-35 keV	Powder X-ray diffraction (PXRD) in Debye-Scherrer geometry using 2D area detector. Sample spinner in horizontal and vertical geometry. Rotation stage in vertical geometry. Sample temperature from 90 K to 500 K 2D PXRD and XRF mapping using continuous and step scans. Total scattering, SDD~95mm, E=35 keV, Qmax~20Å^1.
FemtoMAX	SAXS, WAXS, Scattering, vis fluorescence	1.8-12 keV	Scattering set-up (SAXS, WAXS) Air or He-environment Scattering set-up (in vacuum). Limited scattering range +/-10 degrees horisontal 0-40 degrees vertical Vacuum better than 1E-7 mBar; 2E-6 with Pilatus connected to vacuum; Cryocooling 40K for grazing incidence samples Tilt range +/- 0.5 degrees Wedges available on request to match Bragg angle. No cryocooling with wedges. Tilt platform 0-15 degrees (wedges available on request) Air +/-20 mm translation range Cryostream for LN2 available (performance untested) Life-time measurement by visible fluorescence detection following X-ray excitation
FinEstBeAMS	XPS, NEXAFS, Ion TOF, PEPICO/NIPICO, photoluminescence, UPS, ARPES	4.6-1300 eV	High-resolution photoelectron, TOF and coincidence spectroscopy of gaseous samples Time-resolved photoluminescence spectroscopy XPS, NEXAFS, UPS & ARPES of solid samples
FlexPES	PES, XAS or NEXAFS, Multi-coincidence	40-1500 eV	PES and NEXAFS on solid samples, NEXAFS in partial electron and partial fluorescence yield PES on low-density matter samples using liquid jet setup, molecular jet source, gas cell or magnetron-based source for metal particle beams COLTRIMS/multi-coincidence spectroscopy with single bunch mode
			Veritas B (open port)

Beamline	Techniques	Energy	Capabilities available to users
ForMAX	SWAXS, microtomography	8-25 keV	Early commissioning: Full-field microtomography, without beam-expanding optics based on CRLs. Small- and/or wide-angle x-ray scattering (SWAXS). Scanning SWAXS imaging, without microfocusing optics based on CRLs. Combined full-field microtomography and SWAXS.
HIPPIE	APXPS	250-2200 eV	Catalysis cell: APXPS of solid-gas interfaces, up to 30 mbar, for catalysis and surface science experiments Liquid/electrochemistry cell: APXPS of solid-liquid (dip-and-pull setup) and gas-liquid (liquid jet setup) interfaces up to 30 mbar, for electrochemistry, energy, environmental, and atmospheric science Polarization modulated infrared reflection absorption spectrometer for detection of reaction intermediate species on surfaces simultaneously with APXPS in catalysis cell
MAXPEEM	SPELEEM	30-1500 eV	SPELEEM (micro-LEED, PED, micro-ARPES, XMCD)
MicroMAX	MX	5 – 25 keV	Early commissioning: Rotational crystallography, monochromatic beam, fixed energy, sample changer Serial crystallography - fixed target and injector, monochromatic or wide bandwidth (0.3%; 1%)
NanoMAX	Scanning X-ray microscopy, coherent imaging	6-28 keV	Scanning X-ray diffraction and coherent imaging in Bragg geometry Forward-scatter ptychography and CDI XRF mapping in 2D
SoftiMAX	STXM	275 - 1600 eV	STXM at absorption edges between 275 - 1600 eV, with spatial resolution between 22-60 nm, depending on energy range and sample properties. Ptychography at absorption edges between photon energies 700 - 1600 eV, with illumination spot size between 22-60 nm in focus, depending on energy range and sample properties. Circularly polarized x-rays in both helicities are available in addition to the default linear horizontal polarization in STXM and Ptychography modes. Expert commissioning: STXM, Ptychography and X-ray Fluorescence imaging (XRF) at absorption edges between 1.6-2.5 keV, with illumination spot size of about 60 nm (resolution limit in STXM and XRF modes).

Beamline	Techniques	Energy	Capabilities available to users
SPECIES	APXPS / RIXS	30-1500 eV	Standard cell: APXPS up to 20 mbar, for catalysis, redox studies, and surface science ALD cell: APXPS for in-situ and operando ALD experiments at pressures up to 20 mbar RIXS using GRACE spectrometer (emission energy range 50-650 eV, only linear polarization horizontally and vertically). Solid samples only. LN2-sample cooling available, 4-axis manipulator.
Veritas	RIXS	275-1500 eV	Mid-range performance RIXS, solid samples, LN2 cooled samples, linear polarization (horizontal and vertical), XAS (MCP and photodiode), sample scanning Veritas B (open port)

Appendix 3. Beamline scope completion and availability for users

Beamline	Functionality	Available to users
Balder	X-ray absorption spectroscopy (XANES and EXAFS) in transmission and fluorescence modes	**Yes**
	X-ray Emission Spectroscopy (XES)	Available for commissioning experts Q1 2023 (General users)
	X-ray Diffraction (XRD)	Available for commissioning experts Q1 2023 (General users)
BioMAX	X-ray macromolecular crystallography with SAD and MAD	**Yes**
Bloch	Angle resolved photoelectron spectroscopy (ARPES) using linear vertical or horizontal polarised light in the range 10-1000 eV	**Yes**
	Online scanning tunneling microscopy (STM), 50K - 300K	
	Spin-ARPES	Available for commissioning experts Q1 2023 (General users)
CoSAXS	Solution/soft matter conventional SAXS & bio SAXS	**Yes**
	Time resolved experiments	
	WAXS	Q3 2022 (General users)
	XPCS	To be determined
DanMAX	2D PXRD mapping	**Yes**
	Full field imaging and tomography	Q1 2023 (Commissioning experts) Q3 2023 (General users)
	High resolution diffractometry (HERDi)	To be determined
	Single crystal X-ray diffraction (SINCRYS) endstation	To be determined
FemtoMAX	Scattering set-up (SAXS, WAXS) in vacuum, Air or He sample environments	**Yes**
	Crystallography and grazing incidence X-ray diffraction.	
	Excitation 400 nm – THz radiation.	
	Time-resolved X-ray induced fluorescence measurements.	
	Time resolution 500 fs for scanning measurements, <200 fs for single-shot.	

Beamline	Functionality	Available to users
FinEstBeAMS	Gas-Phase Endstation: Photoelectron and Auger electron spectroscopy Ion time-of-flight mass spectrometry Photoelectron-photon coincidence (PEPICO) and negative-ion/positive-ion coincidence (NIPICO) X-ray absorption	**Yes**
	Photoluminescence endstation: Photoluminescence spectroscopy of solid samples	
	Solid state endstation: X-ray photoelectron spectroscopy Angle-resolved photoelectron spectroscopy (ARPES) Near edge X-ray absorption fine structure (NEXAFS)	
FlexPES	High-resolution photoelectron spectroscopy (PES) and X-ray absorption spectroscopy (XAS or NEXAFS) on solid samples	**Yes**
	High-resolution PES and COLTRIMS/Multi-coincidence spectroscopy on low density matter (LDM) samples	
ForMAX	Full-field microtomography	Q1 2023 (Commissioning experts) Q3 2023 (General users)
	Small- and/or wide-angle x-ray scattering (SWAXS)	
	Combined full-field microtomography and SWAXS	
HIPPIE	APXPS of solid-gas, solid-liquid and gas-liquid interfaces for catalysis, electrochemistry, energy, environmental, and atmospheric science	**Yes**
	HIPPIE B branch	Q4 2023 (Commissioning experts) Q1 2024 (General users)
MAXPEEM	Soft X-ray SPELEEM (micro-LEED, PED, micro ARPES, XMCD microscopy)	**Yes**
MicroMAX	Fixed target serial crystallography	Q4 2022 (Commissioning experts) Q2 2023 (General users)
NanoMAX	Scanning X-ray diffraction and coherent imaging in Bragg geometry	**Yes**
	Forward ptychography and CDI	
	X-ray fluorescence mapping in 2D	
	Forward and fluorescence ptycho-tomography	
	Fourier Zoneplate (FZP) endstation	Available for commissioning experts Q4 2022 (General users)

Beamline	Functionality	Available to users
SoftiMAX	STXM	**Yes**
	Forward ptychography (basic)	
	XMCD Microscopy (basic)	
	Coherent X-ray imaging (CXI)	To be determined
SPECIES	APXPS and in-situ ALD experiments up to 20 mbar	**Yes**
	RIXS experiments	
Veritas	NEXAFS experiments	**Yes**
	Open port experiments	
	RIXS experiments	Q2 2022 (General users)

Appendix 4. 2021 Funding, costs, and results

2021 MAX IV Operating Budget

Final accounts by 2021-12-31

	(MSEK)			
FUNDING	**Actuals**	**Budget**	**Diff**	**Comment**
Research council	360.0	360.0	.0	
Vinnova	15.0	15.0	.0	
Formas	5.0	5.0	.0	
Swedish universities contribution	50.0	50.0	.0	
Lund University	63.4	60.8	2.6	
Finland's contribution to Ops	3.6	3.6	.0	
Estonia's contribution to Ops	.6	.0	.6	A
Industrial beamtime and services	4.1	2.0	2.1	B
Other income	3.6	5.2	-1.6	C
TOTAL FUNDING	**505.3**	**501.6**	**3.7**	

COST	**Actuals**	**Budget**	**Diff**	**Comment**
Rent	-70.8	-72.3	1.4	A
Facility cost	-23.1	-25.9	2.8	
Electricity	-22.3	-22.5	.2	B
Lund University overhead	-24.0	-24.0	.0	
Decommissioning MAX IV	-1.0	-1.0	.0	
Staff	-87.2	-77.9	-9.3	C
Central Project Office	-3.4	-2.7	-.7	D
Accelerators (AFSG, RF, AccDev, Ops)	-5.4	-6.9	-1.4	
Life science beamlines	-34.7	-37.5	2.8	E
LP3 - Lund Protein Production Platform	-.5	-.5	.0	
Physical science beamlines	-43.2	-41.7	-1.6	F
DanMAX	-2.0	-3.3	1.3	
IT & Controls	-42.6	-43.4	.8	G
LUNARC	-.9	-3.5	2.6	H
Engineering I & II	-38.7	-48.2	9.5	I
Safety	-7.8	-9.3	1.5	
Admin support (FIOS, HR, Procur, Legal)	-6.8	-6.6	-.2	
User Office, IRO, COM, HO	-1.6	-3.6	2.0	
Accelerators upkeep and dev.	-12.3	-15.2	2.8	J
Beamline upkeep and dev.	-.7	-1.5	.8	J
Building infrastructure upkeep and dev.	-9.3	-11.3	2.0	J
Beamline office & Insertion Device	-2.2	-4.3	2.2	
Swedish universities in-kind contribution	-11.8	-8.0	-3.8	K
Management contingency	-.6	-5.0	4.4	L
TOTAL COST	**-453.0**	**-475.9**	**20.0**	
Result (Funding-Cost)	**52.3**	**25.8**	**23.7**	
MAX IV co-funding research grants	-.8	-1.1		
Indirect cost research grants	3.9	3.9		
RESULT INCL. EXTERNAL PROJECTS	**55.4**	**28.7**	**26.7**	
Upkeep - allocations VR grant	-18.6	-18.6	.0	M
Upkeep - use of VR allocated grant	.7	1.5	-.8	
Change in undepreciated funds	-58.1	-31.0	-27.1	N
TOTAL	**-20.6**	**-19.4**	**-1.2**	**O**

Appendix 5. 2021 Publications

First Author	TITLE	JOURNAL	DOI
Afzali-Far, B.	Data analysis, spatial metrology network, and precision realignment of the entire MAX IV linear accelerator	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	10.1016/j.nima.2021.165267
Grabski, Marek	Commissioning and operation status of the MAX IV 3 GeV storage ring vacuum system	JOURNAL OF SYNCHROTRON RADIATION	10.1107/S1600577521002599
Olsson, DK	Studies on Transverse Resonance Island Buckets in third and fourth generation synchrotron light sources	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH	10.1016/j.nima.2021.165802
Qin, Weilun	The FEL in the SXL project at MAX IV	JOURNAL OF SYNCHROTRON RADIATION	10.1107/S1600577521003465
Tavares, PF	Beam-based characterization of higher-order-mode driven coupled-bunchinstabilities in a fourth-generation storage ring	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH	10.1016/j.nima.2021.165945
Bocharov, Dmitry	Study of High-Temperature Behaviour of ZnO by Ab Initio Molecular Dynamics Simulations and X-ray Absorption Spectroscopy	MATERIALS	10.3390/ma14185206
Dalgaard, Kirstine Junker	Local structure of Nb in superconducting Nb-doped Bi2Se3	PHYSICAL REVIEW B	10.1103/PhysRevB.103.184103
Frank, Sara	Exploring the influence of atomic level structure, porosity, and stability of bismuth(iii) coordination polymers on electrocatalytic CO2 reduction	JOURNAL OF MATERIALS CHEMISTRY A	10.1039/d1ta06564e
Konieczna, Hanna	Solvation and coordination chemistry of manganese(II) in some solvents. A transfer thermodynamic, complex formation, EXAFS spectroscopic and crystallographic study	POLYHEDRON	10.1016/j.poly.2020.114961
Li, Jinzhao	20.8% Slot-Die Coated MAPbI(3) Perovskite Solar Cells by Optimal DMSO-Content and Age of 2-ME Based Precursor Inks	ADVANCED ENERGY MATERIALS	10.1002/aenm.202003460
Lu, Changyong	High affinity lanthanum doped iron oxide nanosheets for phosphate removal	CHEMICAL ENGINEERING JOURNAL	10.1016/j.cej.2021.130009
Micheal Raj, P	Fabrication and Characterisation of a Silicon-Borosilicate Glass Microfluidic Device for Synchrotron-based Hard X-ray Spectroscopy Studies	RSC ADVANCES	10.1039/D1RA05270E
Shu, Rui	Influence of Metal Substitution and Ion Energy on Microstructure Evolution of High-Entropy Nitride (TiZrTaMe)N1-x (Me = Hf, Nb, Mo, or Cr) Films	ACS APPLIED ELECTRONIC MATERIALS	10.1021/acsaelm.1c00311
Sjöberg, S	Microbe-mediated mn oxidation - a proposed model of mineral formation	MINERALS	10.3390/min11101146
Thrane, Joachim	Highly Stable Apatite Supported Molybdenum Oxide Catalysts for Selective Oxidation of Methanol to Formaldehyde: Structure, Activity and Stability	CHEMCATCHEM	10.1002/cctc.202101220
van Genuchten, C. M.	Decoupling of particles and dissolved iron downstream of Greenlandic glacier outflows	EARTH AND PLANETARY SCIENCE LETTERS	10.1016/j.epsl.2021.117234

First Author	TITLE	JOURNAL	DOI
Khanin, Vasilii	Exciton interaction with Ce3+ and Ce4+ ions in (LuGd)(3)(Ga, Al)(5)O-12 ceramics	JOURNAL OF LUMINESCENCE	10.1016/j.jlumin.2021.118150
Gustavsson, Nadja	Correlative optical photothermal infrared and X-ray fluorescence for chemical imaging of trace elements and relevant molecular structures directly in neurons	LIGHT-SCIENCE & APPLICATIONS	10.1038/s41377-021-00590-x
Aggarwal, S	protocol for production of perdeuterated OmpF porin for neutron crystallography	PROTEIN EXPRESSION AND PURIFICATION	10.1016/j.pep.2021.105954
Asthana, Pooja	Structural insights into the substrate-binding proteins Mce1A and Mce4A from Mycobacterium tuberculosis	IUCRJ	10.1107/S2052252521006199
Baerentsen, Rene	Structural Basis for Regulation of Toxin Activity via Dual Phosphorylation in the Tripartite HipBST Toxin-Antitoxin System	FASEB JOURNAL	10.1096/fasebj.2021.35.S1.02694
Bavnhoj, Laust	Molecular mechanism of sugar transport in plants unveiled by structures of glucose/H+ symporter STP10	NATURE PLANTS	10.1038/s41477-021-00992-0
Cassidy, Andrew	A mechanism for ageing in a deeply supercooled molecular glass	CHEMICAL COMMUNICATIONS	10.1039/d1cc01639c
Cellini, Andrea	The three-dimensional structure of Drosophila melanogaster (6-4) photolyase at room temperature	ACTA CRYSTALLOGRAPHICA SECTION D-STRUCTURAL BIOLOGY	10.1107/S2059798321005830
Di Fruscia, Paolo	Fragment-Based Discovery of Novel Allosteric MEK1 Binders	ACS MEDICINAL CHEMISTRY LETTERS	10.1021/acsmedchemlett.0c00563
Ernits, Karin	Structural Insight into a Yeast Maltase-The BaAG2 from Blastobotrys adeninivorans with Transglycosylating Activity	JOURNAL OF FUNGI	10.3390/jof7100816
Espeland, Ludvik Olai	An Experimental Toolbox for Structure-Based Hit Discovery for P. aeruginosa FabF, a Promising Target for Antibiotics	CHEMMEDCHEM	10.1002/cmdc.202100302
FitzGerald, Edward A.	Discovery of fragments inducing conformational effects in dynamic proteins using a second-harmonic generation biosensor	RSC ADVANCES	10.1039/d0ra09844b
Gysel, Kira	Kinetic proofreading of lipochitooligosaccharides determines signal activation of symbiotic plant receptors	PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA	10.1073/pnas.2111031118
Haddad Momeni, M	Discovery of fungal oligosaccharide-oxidising flavo-enzymes with previously unknown substrates, redox-activity profiles and interplay with LPMOs.	NATURE COMMUNICATIONS	10.1038/s41467-021-22372-0
Hasan, Mahmudul	The structure of human dermatan sulfate epimerase 1 emphasizes the importance of C5-epimerization of glucuronic acid in higher organisms	CHEMICAL SCIENCE	10.1039/d0sc05971d
Kalyani, DC	A homodimeric bacterial exo-beta-1,3-glucanase derived from moose rumen microbiome shows a structural framework similar to yeast exo-beta-1,3-glucanases.	ENZYME AND MICROBIAL TECHNOLOGY	10.1016/j.enzmictec.2020.109723

First Author	TITLE	JOURNAL	DOI
Kelpsas, Vinardas	Neutron structures of Leishmania mexicana triosephosphate isomerase in complex with reaction-intermediate mimics shed light on the proton-shuttling steps	IUCRJ	10.1107/S2052252521004619
Kmezik, C	A polysaccharide utilization locus from the gut bacterium Dysgonomonas mossii encodes functionally distinct carbohydrate esterases.	JOURNAL OF BIOLOGICAL CHEMISTRY	10.1016/j.jbc.2021.100500
Koruza, K	Biophysical Characterization of Cancer-Related Carbonic Anhydrase IX	INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES	10.3390/ijms21155277
Krska, Daniel	Structural and Functional Analysis of a Multimodular Hyperthermostable Xylanase-Glucuronoyl Esterase from Caldicellulosiruptor kristjansonii	BIOCHEMISTRY	10.1021/acs.biochem.1c00305
Lima, GMA	FragMAXapp: crystallographic fragment-screening data-analysis and project-management system	ACTA CRYSTALLOGRAPHICA SECTION D	10.1107/S2059798321003818
Marcos-Torres, FJ	The bacterial iron sensor IdeR recognizes its DNA targets by indirect readout	NUCLEIC ACIDS RESEARCH	10.1093/nar/gkab711
Martelli, G	N-Thio-beta-lactams targeting L,D-transpeptidase-2, with activity against drug-resistant strains of Mycobacterium tuberculosis.	CELL CHEMICAL BIOLOGY	10.1016/j.chembiol.2021.03.008
Mazurkewich, Scott	Structure of a C1/C4-oxidizing AA9 lytic polysaccharide monooxygenase from the thermophilic fungus Malbranchea cinnamomea	ACTA CRYSTALLOGRAPHICA SECTION D-STRUCTURAL BIOLOGY	10.1107/S2059798321006628
Molina, Rafael	Structural basis of cyclic oligoadenylate degradation by ancillary Type III CRISPR-Cas ring nucleases	NUCLEIC ACIDS RESEARCH	10.1093/nar/gkab1130
Nadeem, Aftab	A tripartite cytolytic toxin formed by Vibrio cholerae proteins with flagellum-facilitated secretion	PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA	10.1073/pnas.2111418118
Pallesen, Jakob S.	Deconstructing Noncovalent Kelch-like ECH-Associated Protein 1 (Keap1) Inhibitors into Fragments to Reconstruct New Potent Compounds	JOURNAL OF MEDICINAL CHEMISTRY	10.1021/acs.jmedchem.0c02094
Ramos, Joao	Structural insights into protein folding, stability and activity using in vivo perdeuteration of hen egg-white lysozyme	IUCRJ	10.1107/S2052252521001299
Ramos, Joao	The impact of folding modes and deuteration on the atomic resolution structure of hen egg-white lysozyme	ACTA CRYSTALLOGRAPHICA SECTION D-STRUCTURAL BIOLOGY	10.1107/S2059798321010950
Rehling, D	Crystal structures of NUDT15 variants enabled by a potent inhibitor reveal the structural basis for thiopurine sensitivity.	JOURNAL OF BIOLOGICAL CHEMISTRY	10.1016/j.jbc.2021.100568
Schriever, Karen	Engineering of Ancestors as a Tool to Elucidate Structure, Mechanism, and Specificity of Extant Terpene Cyclase	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	10.1021/jacs.0c10214
Sprenger, J	Guest-protein incorporation into solvent channels of a protein host crystal (hostal)	ACTA CRYSTALLOGRAPHICA SECTION D	10.1107/S2059798321001078
Stopamo, Fredrik Gjerstad	Characterization of a lytic polysaccharide monooxygenase from Aspergillus fumigatus shows	JOURNAL OF BIOLOGICAL CHEMISTRY	10.1016/j.jbc.2021.101421

First Author	TITLE	JOURNAL	DOI
	functional variation among family AA11 fungal LPMOs		
Talibov, Vladimir O.	Discovery of an Allosteric Ligand Binding Site in SMYD3 Lysine Methyltransferase	CHEMBIOCHEM	10.1002/cbic.202000736
Vella, Peter	A FabG inhibitor targeting an allosteric binding site inhibits several orthologs from Gram-negative ESKAPE pathogens	BIOORGANIC & MEDICINAL CHEMISTRY	10.1016/j.bmc.2020.115898
Venskutonyte, Raminta	Structural characterization of the microbial enzyme urocanate reductase mediating imidazole propionate production	NATURE COMMUNICATIONS	10.1038/s41467-021-21548-y
Zhang, SM	NUDT15-mediated hydrolysis limits the efficacy of anti-HCMV drug ganciclovir	CELL CHEMICAL BIOLOGY	10.1016/j.chembiol.2021.06.001
Jensen, Maja	High-resolution macromolecular crystallography at the FemtoMAX beamline with time-over-threshold photon detection	JOURNAL OF SYNCHROTRON RADIATION	10.1107/S1600577520014599
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Caldararu, Octav	Exploring ligand dynamics in protein crystal structures with ensemble refinement	ACTA CRYSTALLOGRAPHICA SECTION D-STRUCTURAL BIOLOGY	10.1107/S2059798321006513
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