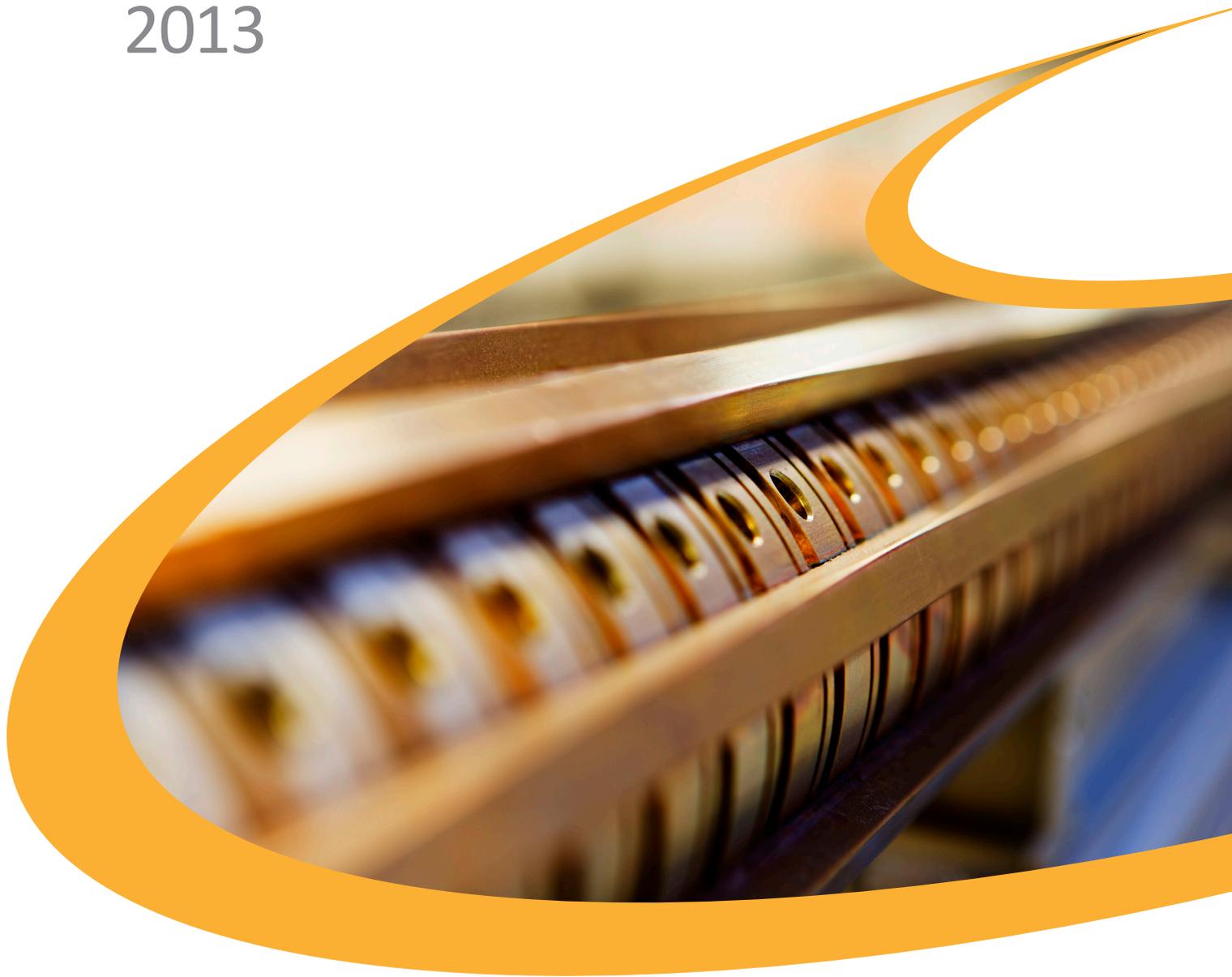


# HIGHLIGHTS AND ACTIVITIES 2013



MAXIV

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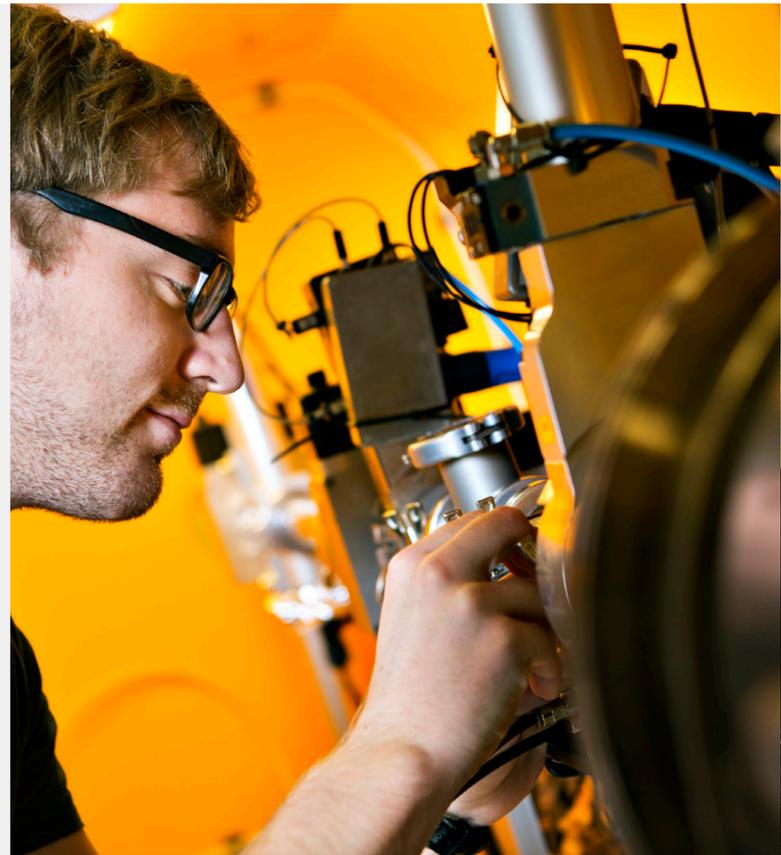
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Front cover photograph:  
Part of the new linac at MAX IV

# MAX IV LABORATORY – MOVING UP STEP BY STEP

MAX IV Laboratory is an organisation on the move. After 25 years of successful science and development at MAX I, II and III we are in the fortunate situation to be able to take the next step. We are building the MAX IV facility. While this is exciting and rewarding it puts our organisation and each one of us to a test. This test has shaped the year 2013.



To begin with the good news: MAX IV Laboratory not only has a bright future as a light source, it also has the money to realize its potential. At the end of 2013 the Swedish Research Council (VR) and Lund University agreed on funding for operations during 2014-2018. For the first time in the history of the lab, there is a multi-annual budget frame allowing strategic planning and a chance to make choices for a long time horizon. This will prove extremely useful when ramping up the staff and the instrumentation for MAX IV. It also allows us to operate MAX II and III until they will be shut down in December 2015. We are grateful for this courageous decision and look forward to investing the money wisely for and with the user community to build up a world-leading research infrastructure.

MAX II and III and their beamlines are still operating with good performance. The science highlights in this report prove it. From fundamental physics over structural biology to environmental science and modern energy materials, MAX II and III still attract a broad and successful user base. At the recent user meeting almost 300 users gathered to report scientific discoveries and to discuss future development at MAX IV. In the need to balance the existing facilities with the project of the future we decided on a statement reflecting the priority: We prioritize MAX IV, our future; we safeguard operations at MAX II & III.

The move to MAX IV requires some restructuring of the laboratory. This includes implementation of group managers with staff responsibility. We are happy to have them in place since the fall and wish them all the best for their challenging tasks. At present they are undergoing training for staff and resource management.

At the MAX IV site things are happening with an amazing pace. The building work is progressing well and is at present a few months ahead of schedule. Since October we are official tenants of the first part, the linac tunnel. The installation of the linac had already started in March 2013 and it is currently in a commissioning phase. In the meanwhile many suppliers are busily working on the components for the two rings and new hardware is arriving every week.

The beamlines for MAX IV are also taking shape, with progress on the design of infrastructure and hutches, as well as many big contracts for beamline components already awarded. In its December meeting the Scientific Advisory Committee deliberated the next four beamlines and unanimously recommended building them. At present the funding for investment is not available, but we will move forward with the design and with hiring staff, to push the cases, expecting the funding to be released as MAX IV proves to be a success.



The plans for the long-term future (2013-2026) were put on paper in a Strategy Report requested by the Swedish Research Council. It describes the full potential of MAX IV as a facility for all of science, reaching far beyond the Swedish user community, to the neighbouring countries. We are looking forward to a time many years from now, when we will be able to look back and can compare this vision to reality. Join us now to get there and be part of looking back then!

Big steps towards internationalisation and partnership with neighbouring countries were made during a workshop and an international conference organised by the Swedish Research Council, as well as in bilateral negotiations between Sweden and Estonia, Denmark, Norway and Finland. And first fruits are there; Estonia and Finland jointly announced funding for FinEstBeaMS, a beamline at the 1.5 GeV ring, dedicated to atomic and molecular physics and aerosols research. This is a good start, which will hopefully be followed by several more internationally co-funded beamlines in the coming years. It will allow exploiting the full potential of the substantial initial Swedish investment and provide world-leading research opportunities for scientists from Sweden and abroad.

The new multi-bend achromat (MBA) idea, which is at the heart of the brightness increase provided by the MAX IV storage rings, is followed with great attention by other facilities all over the world. Many of us travel to other facilities and not only are we encouraged in our work building MAX IV, but we also give advice on upgrades for other sources in Europe, USA, Japan and South America. We are proud to see that all over the world others are following MAX IV, because by definition, that means we are leading.

For me this has been the first full year at MAX IV Laboratory. I have gotten to know the staff and many of the users. I appreciate the hard work and the dedication that drives many people doing science with MAX II & III and working with the MAX IV project. Beyond a doubt this was the most exciting year in my professional life. I am proud of the results that we all have achieved together in 2013 and look forward to 2014. Another year and another step up for MAX IV Laboratory. ■

Thanks to all who contributed,

A handwritten signature in black ink, reading "Christoph Quitmann".

Christoph Quitmann  
Director MAX IV Laboratory

# THIS IS THE MAX IV LABORATORY

The MAX IV Laboratory was established in July 2010 as a Swedish, national laboratory hosted by Lund University. It is the successor of the national laboratory MAX-lab and includes both the operation of the present MAX-lab (MAX I, II, and III rings) and the MAX IV project under realization at Brunns-  
hög in the north-eastern part of Lund.

The formal goals and basic governance of the MAX IV Laboratory were established in an agreement between Lund University (LU), the Swedish Research Council (VR) and VINNOVA in June 2010 and by a related agreement between Lund University and Region Skåne (RS) in July 2010.



The agreement on the MAX IV Laboratory in 2010 has been updated continuously to meet the challenges of the MAX IV project. Staff ramp up, reorganisation and education of the line organisation as well as new administrative routines is all part of the ambition to become an even more professional organisation.

A new strategy report was compiled during 2013 in which the laboratory's goals and strategy up until 2026 was presented. It was sent to the Swedish Research Council and is also available at our web site [www.maxiv.se](http://www.maxiv.se).

The present MAX IV Laboratory is based on MAX-lab's more than 25 years of experience in accelerator physics and storage ring based research. MAX IV, which will be a synchrotron radiation facility with an outstanding performance, is built on this experience. Today about 150 people are employed and the laboratory further benefits by hosting staff from two divisions at Lund University (Division for Accelerator Physics and Division for Synchrotron Radiation Instrumentation) forming the MAX N-fak unit.

The MAX IV laboratory is privileged by having a continuously growing and active user community across a wide range of sciences that since 1985 has contributed to the development of the laboratory. The user community is also heavily engaged in the MAX IV project guaranteeing that it will provide the Swedish, Scandinavian and international scientific communities unique opportunities for experiments by producing the most brilliant synchrotron light in the world.

The laboratory has likewise been important for the development of Swedish front-line positions in several areas of synchrotron radiation based research. This synergetic facility-community relation will be maintained for an optimum development of the MAX IV facility.

The construction of the MAX IV accelerators and accompanying infrastructure is financed by the Swedish Research Council, Lund University, VINNOVA and Region Skåne. The construction is proceeding on schedule with commissioning of the linear accelerator starting in March 2014. Installation of the 3 GeV ring should commence during summer 2014 while the 1.5 GeV ring installation will start half a year later.

Funding for the first thirteen beamlines has been provided by the Knut and Alice Wallenberg Foundation, a joint initiative of Swedish universities, the Swedish Research Council, the Finnish Academy and Estonia. The MAX IV facility can accommodate a total of circa 26 beamlines and the present funding enables construction of beamlines up to half the capacity.

Starting this year, the MAX IV Laboratory is awarding an annual prize to the best PhD thesis based upon results obtained fully or partially at the MAX IV Laboratory. The prize ceremony took place at our annual user meeting and the beautiful statue is handcrafted by Sílvia Forcat, Mechanical Engineer at MAX IV Laboratory.

The first award was given to Dr Ditte Hededam Welner, University of Copenhagen Department of Chemistry, for her thesis "Structural Studies of a NAC Transcription Factor". ■



Four generations of MAX-lab/MAX IV Laboratory directors. From left to right: Nils Mårtensson, Sine Larsen, Ingolf Lindau and Christoph Quitmann. Missing in photo is the first director, Bengt Forkman.



# MAX IV – A GREEN FACILITY



The 17 October 2013 was an important milestone in the MAX IV building project. The key to the first stage of the project was handed over to Lund University and MAX IV Laboratory at a ceremony in the linac hall.

MAX IV is currently being constructed at Brunshög in north-eastern Lund. The construction work is carried out by the contracting company PEAB AB on commission of the future owner, Fastighets AB ML4. FOJAB has designed the buildings while Snøhetta is responsible for the landscape design. The aim is to build a facility that will serve the science well, be environmentally friendly and be an eye catcher in the dynamic north-eastern Lund area. The facility won the category Best Futura Project at MIPIM in March 2014.



### Sustainable thinking all the way

The design and construction of MAX IV are based on the latest techniques and knowledge. The very first BREEAM-SE application, number 001, belongs to MAX IV and we hope to be the first to receive approval. This classification and the one of Green Building relates to the office building but the same high-level environmental standards have been used for the entire facility. To reach the goals, an extensive program for sustainable construction has been implemented. This has for example resulted in led-lights in all of the buildings, demand-controlled ventilation and green roofs that improve insulation, help stabilizing the temperature in the experiment halls while storing and delaying rain water drainage reducing the impact on sewage systems and improving wildlife environment.



*Aerial rendering of the MAX IV exterior architecture and landscaping by FOJAB and Snøhetta. South-west is towards the top of the image.*



from the nearby nature reserve Kungsmarken and from commercially available seeds will be sown on the slopes. And instead of using your ordinary, motorized lawn mower the slopes are planned to be grazed by sheep. Water is an important feature for wildlife and also enhances the biological diversity, and there are rainwater delay ponds for the surface water where wetland vegetation will be introduced.

**A huge project**  
So far 50 000 m<sup>3</sup>, approximately 120 000 tons, of concrete has been poured and 7 000 tons of steel reinforcement bars come to use.

The building project is divided into two stages and four building packages. Each building package has an individual, early access date for start of the MAX IV assembly.

The steel structure for the office building, including the top floor space frames bridging over the large storage ring building, is in place. So is weather proofing of the facades and roofing, excluding the solar panel assembly which will be installed during 2014.

The large experimental building housing the 3 GeV ring is under roof since Christmas 2013. Approximately 90 per cent of the building structure including steel frames, precast concrete elements in the facade and the “halo” is finalised and glazing is rapidly progressing. The eastern extension for the chemistry lab and the extension to contain the NanoMAX beamline is well under way. The building and installation works inside the large experimental building is progressing at a fast and steady pace. So is the building works on the smaller experimental building for the 1,5 GeV ring.

The latest prognosis for the building project points to an earlier completion of all building, installation and landscaping works and thus an advanced final hand over date. Current cost prognosis also point at a cost below the calculated.

A promising cooperation has been established with the Lund city development office, city planning office and technical office regarding infrastructure development in the vicinity of MAX IV. The collaboration is developed mostly around the issues of reduction of vibrations and electromagnetic fields from road traffic, future public transport as well as power and sewage lines. ■

Also the construction process in itself includes goals for sustainability, for example “greener” logistics, low energy consumption, a minimum of waste, waste sorting etc. The ambition is to make MAX IV a sustainable research facility, probably the first of its kind in the world, with accelerators and all technical equipment designed for lowest reasonable power use. The buildings are designed for energy

efficiency and the equipment will be operated using intelligent power management. Electrical power will be bought from renewable sources and the excess heat from the cooling systems will be sold and used in the Lund city district heating and cooling system. The aim is to have a power consumption that corresponds to approximately half of what similar facilities consume.

The landscape around MAX IV follows the high sustainability agenda for the area. For example, all the cut and fill from the excavations are kept on site and are reshaped into a hilly landscape, constructed to reduce vibrations and to maximize the land surface area. This gives room for more grass, flowers, recreational areas, birds and frogs. To further enhance the ecological diversity, a mix of seeds

# MAX IV ACCELERATORS PUSHING THE LIMITS

The accelerators at MAX IV are realized using novel accelerator technology developed at the MAX IV Laboratory. These provide unprecedented performance at lower cost compared to conventional accelerator concepts.

The MAX IV accelerators consist of three main parts; a large ring with a circumference of 528 meters where the electrons are stored at an energy of 3 GeV, a smaller 96 meter circumference ring with an operation energy of 1.5 GeV and a 300 meter long linear accelerator (linac) used to inject electrons into the two rings. The two rings will together house circa 26 beamlines when fully equipped and the linac will be able to generate very short X-ray pulses at the Short Pulse Facility (SPF). The linac design permits future upgrades into a free electron laser (FEL) to meet the growing needs of extremely short and intense X-ray pulses from the scientific community.

The operation of the present facility at MAX-lab will continue until the end of 2015 when the MAX I, II and III accelerators will be shut down and retired.

## The MAX IV linac

The MAX IV linac is the first of the three accelerators that will be operational. Installation and alignment of the linac components started in late spring 2013. All components of the linac were installed during the summer and autumn of 2013 and commissioning of the linac will commence in the mid 2014.

The linac will be used both for injection into the two storage rings, and also as a high brightness injector for the SPF. The

linac has also been designed to handle the high demands of an FEL electron source. In the storage ring injection mode, the linac is operated at 10 Hz with a thermionic radio frequency (RF) gun and the electron bunches are extracted from the linac at either 1.5 GeV or 3 GeV to reach the respective storage ring. For the Short Pulse mode the linac will operate at 100 Hz with a high brightness photo cathode gun.

Two special magnetic structures in the linac compress the electron bunches such that their time duration is ultra-short, on the order of 100 fs. One quite unique feature of the MAX IV linac bunch compressors is that they use the configuration of dipole, quadrupole and sextupole magnets to shape the electron bunch time profile. This solution is much cheaper, more reliable and simpler than conventional bunch compressors in which an extra accelerating structure, operating at a higher frequency, is used. Simulation results can be seen in Figure 2.

The acceleration is performed in 39 linac sections. These 39 linac sections are powered by 18 radiofrequency modulators and klystron units. It is in these units that the very high power needed to accelerate the electrons is created, see Figure 1.

The installations and subsystem tests of the linac has been on schedule (although not without complications). If all continues as planned we should have electrons accelerated to 3 GeV by summer of 2014.

## The MAX IV Storage Rings

Work on the MAX IV rings is progressing according to plan with significant achievements during 2013. All major procurements of equipment have been done, prototypes for critical subsystems have been built, tested and approved

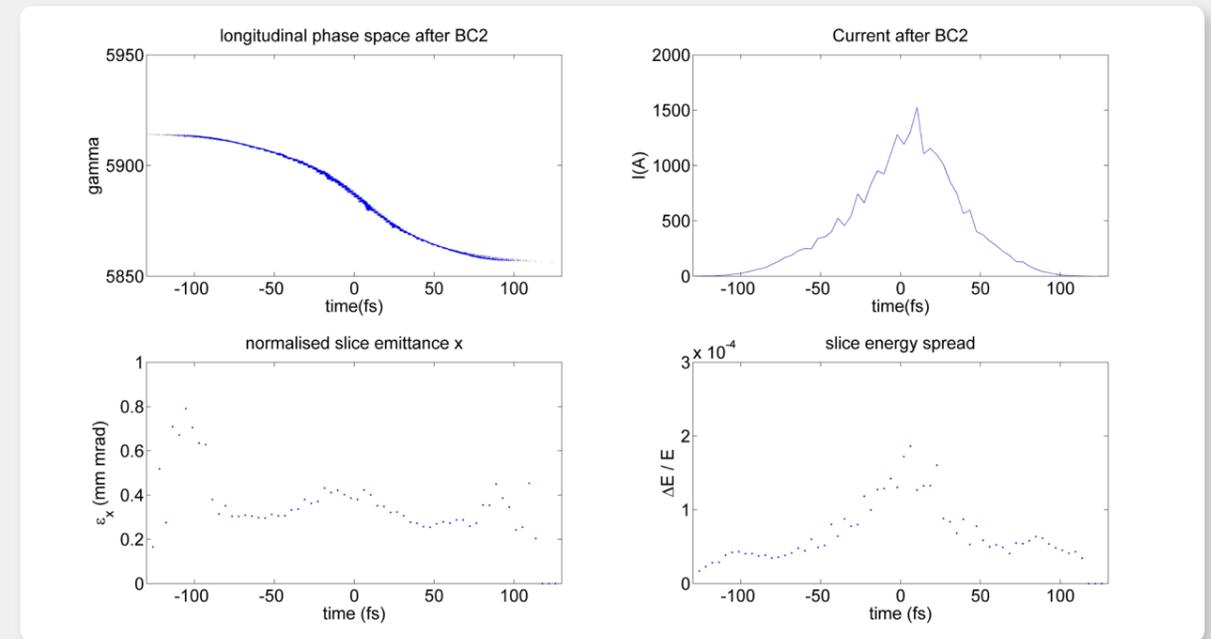


Figure 2. Simulation of an SPF pulse from the MAX IV linac.

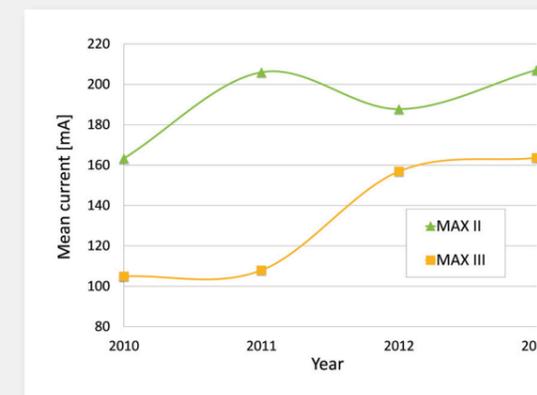


Figure 3. The mean annual current in MAX II and III.

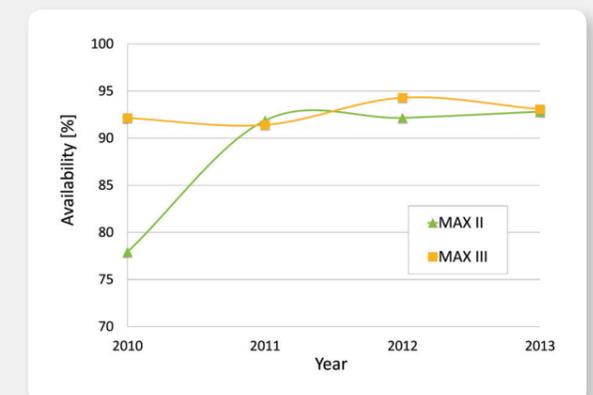


Figure 4. The availability of beam to users at MAX II and III.

## MAX IV linac layout

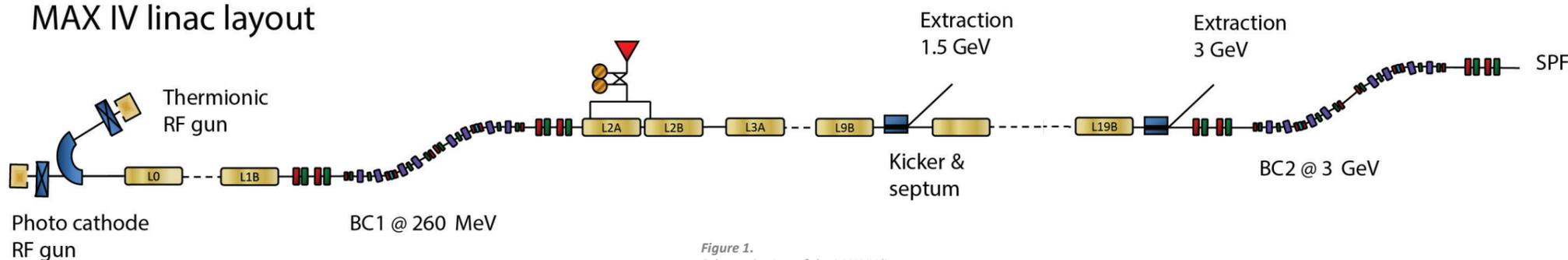


Figure 1. Schematic view of the MAX IV linac.



The view through the linac tunnel showing part of the installed linac.



A quadrupole magnet for the linac at MAX IV.

and series production of components for the 3 GeV ring is now well under way.

Among the most important components in the rings are the magnets that are responsible for guiding and focussing the electrons around the ring. A novel technology developed at the MAX IV Laboratory whereby several compact magnets are housed in the same iron block allows the implementation of the so-called multibend achromat (MBA) lattice. The technology has attracted significant worldwide attention and will be copied at several other synchrotrons in the coming years [1].

The 3 GeV ring will include 140 of these blocks while the smaller 1.5 GeV ring will house 12 blocks. Some important milestones reached during 2013 include the demonstration of the tight mechanical tolerances required for the machining of the magnet blocks and the validation of magnetic measurement benches which allow a precise characterization of the magnetic field strength. At the end of 2013 series production of the magnets progressed at full speed.

Another technology novel to synchrotrons is the vacuum chamber solution in the large ring. Ultrahigh vacuum will be achieved by a special coating of reactive metals (so called NEG or non-evaporable getter coating) on the inside of the chambers. A collaboration agreement has been established with CERN, where the technique was originally developed, to allow the development of NEG coating procedures for the most complex geometries (the ones close to the synchrotron light extraction ports) and successful coating of such chambers was demonstrated in 2013.

Work on dipole pulsed magnets for injection from the linac into the two rings (done in collaboration with Budker Institute in Novosibirsk) has proceeded from detailed engineering design to fabrication of the components. At the same time, the development of multipole injection

kickers, in collaboration with the synchrotrons SOLEIL and BESSY, has achieved the stage of detailed engineering design. These kickers will use solid state pulsers and allow nearly transparent top-up of the stored current in both rings, i.e. the influence of the injection upon stored electrons will be minimal. One important feature of the chosen design is that the same mechanical layout can be used for the 3 GeV and 1.5 GeV rings as well as for the SOLEIL kicker, with a significant reduction in development costs and time.

Finally, after successful conditioning of a pre-series 100 MHz radio-frequency (RF) cavity at the end of 2012, series production was approved and initiated as planned, and all cavities were delivered by the end of 2013. The high power RF plant contracts have all been signed including transmitters, circulators and transmission line systems. The same type of amplifier tubes (tetrodes) as currently used in the MAX II ring have been chosen and will be able, in the final configuration, to produce up to 120 kW per cavity.

#### MAX II & III - Still Improving Their Performance

The MAX IV Laboratory is currently operating three synchrotron rings at MAX-lab. The first ring MAX I has ever since the start in 1986 played a prominent role in stimulating and developing Swedish synchrotron radiation research. Furthermore, some pioneering work in accelerator physics research has been performed at this low energy, 550 MeV, second generation light source. See for example [2-6]. However, the MAX III ring has now taken over the synchrotron radiation task and the MAX I ring is currently used as a pulse-stretcher for photo induced nuclear physics experiments only.

The MAX II ring is a third generation synchrotron radiation source of 90 meter circumference with an operating energy of 1.5 GeV. Even though operating at relatively low energy, MAX II serves seven hard X-ray experimental stations

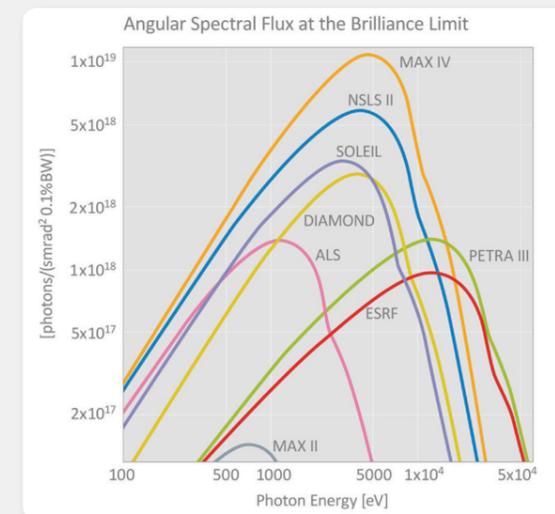
along with several soft X-ray and vacuum ultraviolet (VUV) experiments. The hard X-rays are produced by three high-field multi-pole wigglers.

The MAX II ring has been operating very well during the whole 2013 exceeding the mean current and availability (the fraction of beamtime with available beam for the users) figures from former years, see Figure 3 and 4. Furthermore, the electron beam position stability is in the micrometer range.

In contrast to the rings at MAX IV, electrons are injected into MAX II at an energy (400 MeV) lower than the operation energy and then accelerated in the ring. Injections are carried out twice a day and are scheduled to take one hour. The injections would in principle bring the availability down to 92 % (2 hours out of the 24 per day). However,

since our operators are skillfully handling all actions, the injection time is usually shorter, which fully compensates the downtime due to unexpected failures. The 93 % availability figure for 2013 could actually be interpreted as if we delivered 100 % beam time! Each injection inserts 275 mA of circulating current and some 170 mA remains at the next injection. The mean stored beam current was 207 mA for 2013.

The MAX III ring is a small, 36 meter circumference, third generation light source, serving VUV and infrared (IR) experiments. Its energy is 700 MeV and injected five times per day it also relies on a low energy injection scheme. Each injection is roughly 15 minutes, which ideally gives a stored beam availability of around 95%. 2013 we reached an availability of 93% and a mean stored beam current of 164 mA, see Figure 3 and 4. ■



Brilliance of MAX IV compared to those of other synchrotron facilities across the world.



Cavities waiting to be installed in the 3 GeV ring at MAX IV.

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1. Nature 501, 148 (2013); <http://www.nature.com/news/ultimate-upgrade-for-us-synchrotron-1.13721>
2. P. Röjssel, Nucl. Instr. and Meth. A 343, 374 (1994).
3. Å. Andersson, S. Werin, T. Meinander, A. Naves de Brito and S. Aksela, Nucl. Instr. and Meth. A 362, 586 (1995).
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# MAX IV BEAMLINES SHINING BRIGHT

The goal of the MAX IV Laboratory is to exploit the excellent MAX IV light sources by constructing 26 state-of-the-art beamlines around the accelerators and tailor them to the needs of a broad user community.

The year 2013 saw some major developments for the MAX IV beamlines. The seven initial beamline projects progressed according to plan and are approaching the installation phase. Meanwhile, the number of funded beamlines increased from seven to thirteen including the first international contribution to MAX IV from Estonia and Finland.

Just over two years have now passed since the MAX IV Laboratory received funding of 562 MSEK from the Knut & Alice Wallenberg Foundation (KAW) and 12 Swedish Universities for the first seven beamlines at MAX IV. This initial beamline project has a clearly defined scope to build state-of-the-art beamlines for a range of scientific fields, see page 18. At the start of the project, many issues were unresolved, for example how several beamlines could be built in parallel, how to ensure the best use of the limited resources at the MAX IV Laboratory, how to organize the individual beamline projects and most importantly how to ensure scope and best possible quality within the available budget.

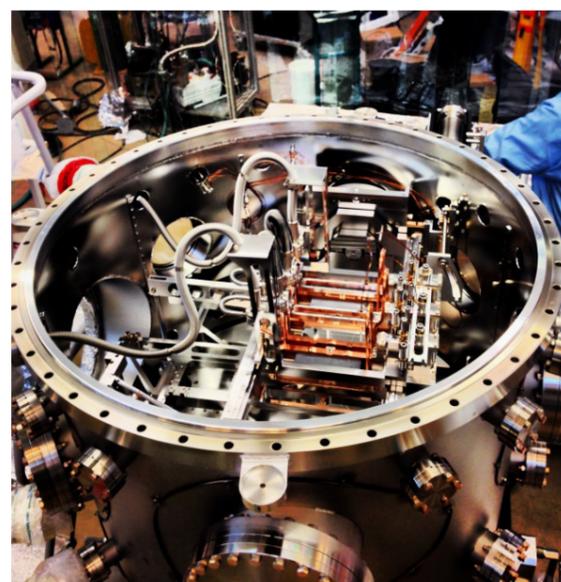
The initial beamlines have since evolved to detailed and externally evaluated designs and the individual beamline projects are progressing according to schedule and budget plans. Some insertion devices have been acquired while the designs of others are being finalized. The procurement of main optical components is either finished or on-going for all beamlines. Call for tenders have been published for a conceptual front end design. Properly defined and standardized solutions for the supporting infrastructure have been developed and implemented.

This progress would not have been possible without the skills and devotion of the individual beamline teams and a well-established beamline project organisation (BPO) [1] with clear mandates and responsibilities for all involved, tools for status and risk analysis, and the fact that a culture has evolved where all beamlines support each other to achieve the common goal of building the best beamlines for MAX IV within the given scope and resources. This model will be put to the test even more in the coming few years with increased emphasis on the installation and commissioning phases for the initial beamlines.

Lately, six more beamlines have been added to the MAX IV portfolio. The first international beamline, FinEstBeaMS for spectroscopy and materials science, has been made possible with funding from Estonia and Finland. The SPECIES beamline, funded by KAW and VR, is currently constructed at the MAX II ring and will be moved to the 1.5 GeV ring at MAX IV.

The second stage of the MAX IV beamline process, Phase IIa, started in December 2012 and involved nine beamline proposals developed from those described in the Strategic Plan 2012-2020 [2]. Following short and intense interactions with the user community, ranking by the Scientific Advisory Committee (SAC) and the Board of the MAX IV Laboratory, an application was submitted to VR in late March 2013 requesting funding for the CoSAXS beamline, the SoftiMAX beamline and a Transfer Package, in total 250 MSEK.

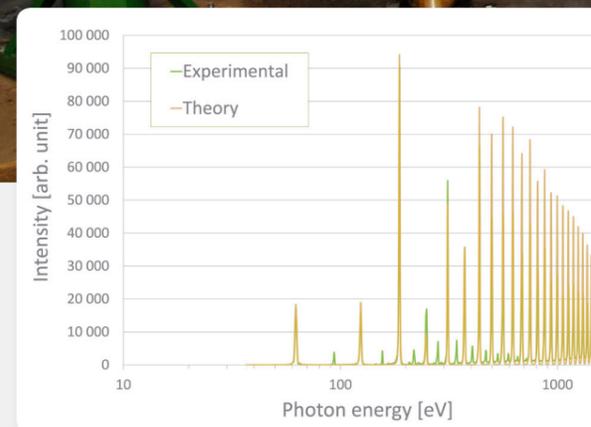
The Transfer Package consists of equipment from MAX II which will be reused to construct two beamlines at MAX IV: FlexPES and MAXPEEM. KAW granted 15 MSEK for the Transfer Package in May 2013. Funding for the Phase IIa beamlines, including the remaining parts of the Transfer Package, was granted by VR in December 2013 bringing the total number of funded beamlines at MAX IV to thirteen. Planning, design and construction of these and any other new beamlines will be accommodated within the established BPO organisation model.



The plane grating monochromator for SPECIES, delivered by FMB Berlin.



The SPECIES EPU in place at MAX II.



First spectrum of the SPECIES EPU compared with the theoretical prediction.

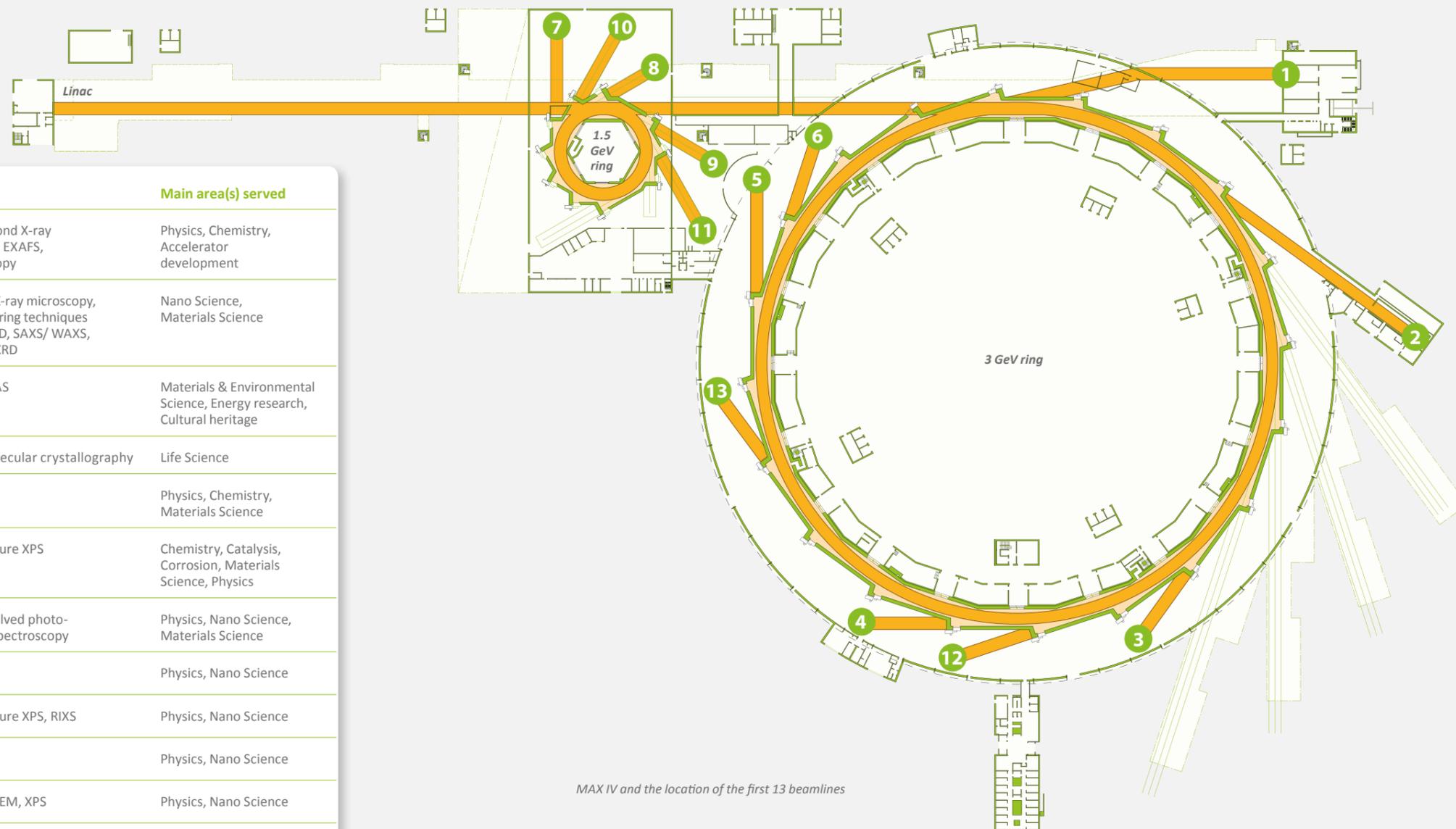
## SPECIES

The SPECIES beamline is currently being assembled at MAX II and commissioning will start at the beginning of 2014. SPECIES will serve two endstations, each at its own branch: An AP-XPS end station and a RIXS spectrometer. Once operational, the beamline is unique in terms of techniques offered in the low energy region.

The insertion device, an elliptically polarizing undulator (EPU), was installed during the Easter shutdown in 2013. The first undulator spectra were recorded in April

2013 after preliminary alignment, and agree well with what is expected from theory. The insertion device is the result of a design project of importance for future MAX IV soft X-ray EPUs and incorporates new concepts for the magnet mounting and end section design. It has an energy range of 27-1200 eV and full polarization control. At present, the monochromator is being installed and alignment of the optical elements has been performed. Control systems are installed in parallel. SPECIES will use the same control technology as the MAX IV beamlines.

The first 13 beamlines planned for construction at MAX IV.



Name	Number	Energy range	Accelerator	Methods	Main area(s) served
FemtoMAX	1	1.8 - 30 keV	linac	Femtosecond X-ray scattering, EXAFS, spectroscopy	Physics, Chemistry, Accelerator development
NANOMAX	2	5 - 15 keV (optimal)	3 GeV ring	Scanning X-ray microscopy, XRF, scattering techniques such as XRD, SAXS/ WAXS, coherent XRD	Nano Science, Materials Science
BALDER	3	4 - 40 keV	3 GeV ring	(in-situ) XAS	Materials & Environmental Science, Energy research, Cultural heritage
BioMAX	4	5 - 25 keV	3 GeV ring	Macromolecular crystallography	Life Science
VERITAS	5	275 - 2000 eV	3 GeV ring	RIXS	Physics, Chemistry, Materials Science
HIPPIE	6	260 - 2000 eV	3 GeV ring	High pressure XPS	Chemistry, Catalysis, Corrosion, Materials Science, Physics
ARPES	7	10 - 1000 eV	1.5 GeV ring	Angle resolved photo-electron spectroscopy	Physics, Nano Science, Materials Science
FinEstBeaMS	8	4 - 1000 eV	1.5 GeV ring	XPS, XAS	Physics, Nano Science
SPECIES	9	30 - 1200 eV	1.5 GeV ring	High pressure XPS, RIXS	Physics, Nano Science
FlexPES	10	30 - 1200 eV	1.5 GeV ring	XPS, XAS	Physics, Nano Science
MAXPEEM	11	30 - 1200 eV	1.5 GeV ring	XPEEM, LEEM, XPS	Physics, Nano Science
CoSAXS	12	5 - 18 keV	3 GeV ring	SAXS/WAXS, XPCS & CDI	Soft matter, Life Science
SoftiMAX	13	250 - 2200 eV	3 GeV ring	CXI & STXM	Physics, Nano Science, Materials Science

### Future Beamlines

The definition and planning of further beamlines at MAX IV is carried out in interaction with existing and future user communities, and with all other stakeholders. This process is fundamental for an efficient exploitation of the full potential of the MAX IV light sources. A full description of the details of this process can be found in the MAX IV Laboratory Strategy Plan 2013-2026 [3].

A series of workshops related to Phase IIb beamlines were initiated by the MAX IV Laboratory during 2013. Organized

by groups from the user community, the workshops focussed on discussions of science cases and/or specific beamlines within the scientific community. Based upon feedback from the workshops and further discussions at a special session at the 2013 Annual Users Meeting, a list of future beamlines was identified and workgroups were formed around each of them. The University Reference Group (URG) was encouraged to submit comments and input about the ranking of the beamlines during the year. The scientific cases were further developed by the workgroups during the autumn and presented to and ranked

by the Scientific Advisory Committee (SAC) at a meeting in December. The SAC suggested the following ranking in their report [4]:

1. MicroMAX
2. MedMAX
3. DiffMAX
4. iMAX

The SAC furthermore found that the case for all of these beamlines is very strong, and that ideally all should be built

as soon as possible. Despite investment funding not being available, it has been decided to move forward with hiring of staff needed to further develop the scientific and technical cases of these beamlines. ■

### References:

- [1] [www.maxlab.lu.se/BPO](http://www.maxlab.lu.se/BPO)
- [2] [www.maxlab.lu.se/sites/default/files/Strategisk%20dok\\_0.pdf](http://www.maxlab.lu.se/sites/default/files/Strategisk%20dok_0.pdf)
- [3] [www.maxlab.lu.se/strategy\\_report](http://www.maxlab.lu.se/strategy_report)
- [4] Report of MAX IV SAC: 4-5 December 2013.

# MAXIMIZING THE SERVICE TO INDUSTRY

The MAX IV Laboratory is committed to actively engage with, and serve the needs of Swedish and international industry by providing tailored solutions and reliable access to its brilliant synchrotron X-ray sources.

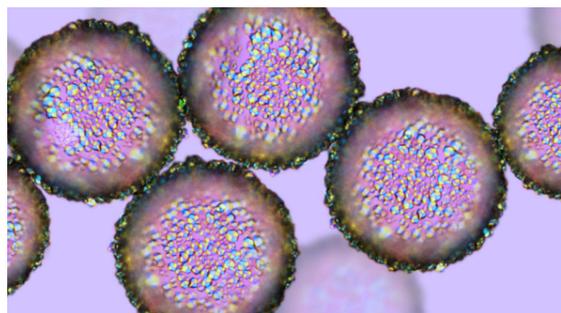
## Our Vision for Industry; Today and Tomorrow

Companies from a wide range of industrial sectors can benefit from the synchrotron X-ray sources at the MAX IV Laboratory to solve R&D problems relating to nearly all types of materials. Examples include the investigation of protein structures by life-science companies and studies of catalytic processes by chemical companies. The Industrial Liaison Office (ILO) at the MAX IV Laboratory [1] assists commercial users with advice on suitable experiments, scheduling of beamtime and analysis of results. It also operates an active outreach programme to inform companies about the advantages of synchrotron radiation.

The MAX IV Laboratory continued to serve industry during 2013 with many companies from the pharmaceutical, chemical, life-sciences and even food sector using the facility, partly through the Science Link project (see next section) and partly on a commercial basis. The ILO was strengthened with staff experienced in industrial R&D and the MAX IV Laboratory Industrial Network Group (MING) was launched. The MING will advise the MAX IV management on all aspects of commercial use of the facility ranging from access modes to experimental infrastructures, support labs and suggestions of beamlines for MAX IV. Together with the stakeholders of MAX IV it will consider various ways of enhancing the general industrial use of the facility for example through targeted research and partnerships between private and academic players. For a list of MING members see the Facts and Figures chapter.

The industrial services at the MAX IV Laboratory were further bolstered through the recruitment of Dr. Tomas

*Drops of emulsion with starch on the surface. Photo: Anna Timgren.*



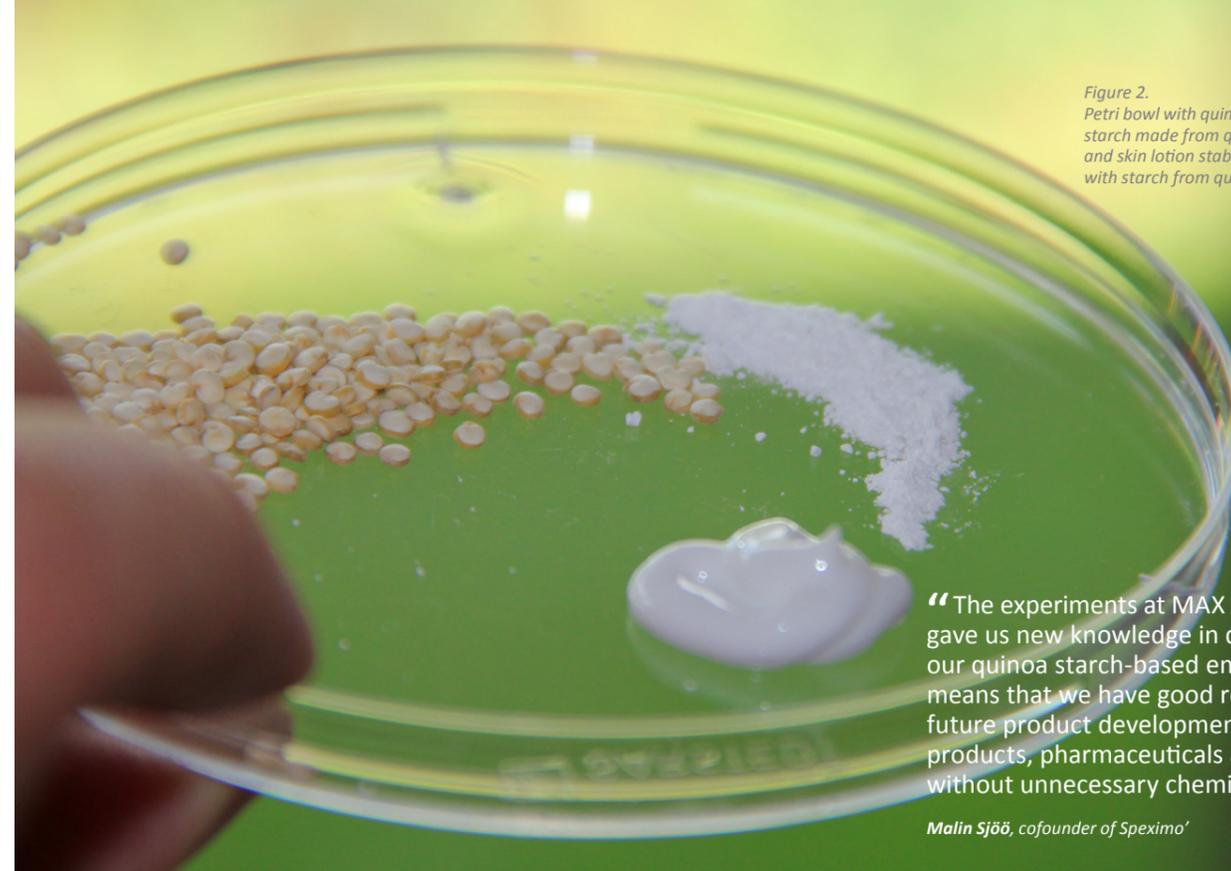
Lundqvist as Director of Life Sciences at MAX IV Laboratory. With a background as Director of Discovery Sciences at AstraZeneca he brings valuable experience of R&D in an industrial setting.

The outreach work towards industry intensified during the year, best exemplified with the organisation of a workshop in October dedicated specifically towards industry. The one-day event, held at the Royal Engineering Academy (IVA) in Stockholm, attracted more than 60 participants from small to global companies. The workshop explored how current synchrotron facilities are used for industrial R&D, and how MAX IV can improve its services in the future. Three keynote speakers from industry, representing pharmaceutical, mechanical engineering and petrochemical research, elaborated on their extensive experience with existing facilities in Europe and world-wide. The workshop was rounded off by presentations from the Swedish high-energy X-ray beam line at Petra III, an update on the Science Link initiative, and summary conclusions by a representative from VINNOVA.

## The Science Link Project

The MAX IV Laboratory is a partner in the Science Link [2] project aimed at attracting companies to becoming regular users at large scale synchrotron and neutron facilities. Active since 2012 it has been able to offer free beamtime for feasibility studies to nearly 50 companies from countries around the Baltic Sea. Many of these companies have since chosen to perform follow-up experiments at the large scale facilities.

Funded through the EU Baltic Sea Region programme 2007-2013 the project includes four large scale facilities; the MAX IV Laboratory, DESY and the Helmholtz centres in Berlin and Geesthacht. Other partners include universities, and publically funded business development agencies. The cooperation between large scale facilities and local organisations in the project has proven a success. In particular Sweden has seen a large influx with 20 interested companies taking up the offer. Science Link has enabled the MAX IV Laboratory to host 15 companies for beamtime from a broad range of industrial sectors including chemicals, the life-sciences, electronics, nanotechnology and the water industry. The project has also enabled the MAX IV Laboratory to



*Figure 2. Petri bowl with quinoa seeds, starch made from quinoa and skin lotion stabilised with starch from quinoa.*

“The experiments at MAX IV Laboratory gave us new knowledge in detail about our quinoa starch-based emulsions. This means that we have good references for future product development of skin care products, pharmaceuticals and foods without unnecessary chemicals.”

*Malin Sjöö, cofounder of Speximo*

broaden its service as more than half of the beamlines at MAX II and MAX III, including some previously never before utilized by commercial users, were accessed by the Science Link companies.

## Skin care products without mess and allergens

The vast majority of skin care products – creams, lotions, sunscreen, etc. are so-called emulsions containing both water and oil in microscopic droplets. To make the emulsions stable, chemicals are added. They make many skin care products unusable by people with allergies and are also an unnecessary burden on the environment.

Speximo is a research-based company that has developed a completely new approach where ordinary food starch is used as a stabilizer instead of chemicals. Today Speximo works with customizing emulsions for the three areas Personal Care, Pharmaceuticals and Food.

Dr. Malin Sjöö is Associate Professor of Food Technology, expert in starch and one of Speximo’s founder. [3] “I worked with other scientists in a project on how to use starch to encapsulate bioactive compounds in foods. We tested the starch from many different plants and discovered that quinoa starch was best at encapsulating the oil in water. We had found a new way of making fine emulsions. This led us on to other uses and cosmetic products was close at hand because they are often just emulsions. It turned out to work better than expected – quinoa-based skin creams goes rapidly into the skin without smudging.” ■

## References:

- [1] [www.maxlab.lu.se/industry](http://www.maxlab.lu.se/industry)
- [2] [www.science-link.eu](http://www.science-link.eu)
- [3] [www.speximo.com](http://www.speximo.com)



**Malin Sjöö**  
CEO, Speximo

**Speximo** develops an environmentally friendly and skin-friendly alternative to stabilizing emulsions used in skin cream. The product contains bio-degradable starch from Quinoa used to separate the oil and the water in the emulsions.

**The company** was founded in Lund in 2012, is based on research carried out at Lund University and gained access to small-angle X-ray scattering (SAXS) beamtime through Science Link during 2013.

**The measurements** were carried out to investigate how the properties of the starch structure differ in the emulsion in comparison to the structure in the aqueous phase.



## SCIENTIFIC HIGHLIGHTS

# EXAMINING PROTEIN STRUCTURES TO FIGHT DISEASE

Structural information on biological macromolecules is an important tool for modern life-science research. It provides deep insight into the chemistry of the molecules studied and is a cornerstone of disciplines stretching from cell biology, biomolecular medicine, biochemistry and more. Recent work at the MAX IV Laboratory MX beamlines as well as the SAXS beamline I911-4 shows the importance of structural information for the understanding of physiology and the development of disease, in particular multiple sclerosis.

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For our nervous system to work fast and reliably, the nerve fibers (axons of neural cells) making up the nervous system are embedded in a sheath of material called myelin.

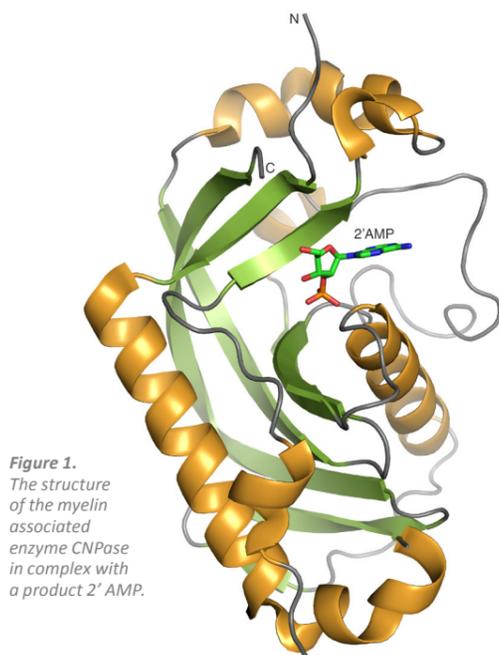
Myelin is a unique biological membrane with dielectric properties that insulate the axons from electrically charged atoms and molecules in the environment. This ensures that signals through the nerve cells can travel faster. The insulation of the long axons by myelin is thought to be required for communication between the brain and distant body parts, like toes and fingers.

The myelin sheath is a multi-layered membrane, rich in lipids and low in water content. Production of myelin starts in the embryo around week 14 and continues after birth through

childhood and adolescence. When the myelin sheath surrounding the axons gets damaged or destroyed, the speed of signals will be slowed down, or signals might not even be received at all. This can lead to an array of problems, including unclear vision, coordination problems or difficulties with bodily functions, such as bladder control. Loss of the myelin sheath, also called demyelination, is one of the characteristics of some neurodegenerative diseases, among which the most well known is multiple sclerosis (MS). Myelin repair is one of the possible therapies for MS; however, no efficient treatment for stimulating repair has yet been established.

A small number of proteins exist that are mainly or only expressed in cells producing the myelin sheath [1]. One of the most abundant myelin proteins is 2',3'-cyclic nucleotide 3'-phosphodiesterase (CNPase), an enzyme anchored to the membrane itself. CNPase amounts to as much as 4% of the total protein found in myelin from the central nervous system. It is thought to play an important role in the formation of the myelin sheath. Mice, in which the protein has been removed (knock-outs), develop serious neurological symptoms at around 3 months of age and die when they are between 6 to 9 months old. Mice with decreased expression levels of CNPase show signs of psychiatric disorders and depression. Although there is still a lot to learn about the exact function of this protein, it may have a role in RNA splicing. Since it has been suggested the latter could play a role in myelin formation, the understanding of myelination at the molecular level may pave the way for possible therapies for MS by myelin repair.

CNPase is member of a family of proteins called 2H phosphodiesterases. The targets of these enzymes are unusual phosphodiester bonds, which they hydrolyze. This type of bond can be found in nucleotides containing 2',3'-cyclic phosphates, 1',2'-cyclic phosphates, or 2',5'-oligoadenylates. Such nucleotides can be found for example in RNA, and 2H phosphodiesterases play important roles in RNA chemistry and function within the cell. Members of the family share similar 3-dimensional structures, consisting of two lobes with the active site between them. The active



**Figure 1.** The structure of the myelin associated enzyme CNPase in complex with a product 2'-AMP.



Marjolein Thunnissen  
Beamline manager I911-MX

PhD in chemistry at Groningen University, Netherlands  
At MAX IV Laboratory since 2001

**The users** at the MX beamlines I911-2 and I911-3 measure diffraction data from crystals of macromolecular molecules. The data is used for the determination of the structure at atomic detail of these macromolecules.

**As the function** of these molecules, e.g. proteins, is closely linked to the structure, this kind of information is very important in modern day (cell) biology, biochemistry and biomedicine and it is an important tool within drug discovery.

**The importance** of this field is illustrated by the many Nobel prizes that has been awarded to scientists within this field, most recently in 2009 and 2012.

sites of the different family members are highly conserved, and it is presumed that the reaction mechanisms of the enzymes are also highly similar.

In CNPase, the phosphodiesterase activity itself is located in the C-terminal domain of the protein, but an additional N-terminal domain, with a hitherto unknown function, is also present. Although the structure of the human CNPase phosphodiesterase domain had been solved previously, no structural data were available for this protein in complex with active site ligands, be it substrates, products or transition states of reaction intermediates. This type of data is required to fully understand the chemistry of CNPase, and will be an important tool for the development of specific inhibitors or modulators. In this work, the C-terminal domain of mouse CNPase was crystallized, and its 3-dimensional structure was solved. The work performed at the macromolecular crystallography (MX) beamlines of the MAX II ring included the structure determination of complexes of mouse CNPase with two different reaction products, NADP<sup>+</sup> and 2'-AMP [2] (Figure 1). These products were produced by soaking the CNPase crystals with its in vitro substrates 2',3'-cNADP<sup>+</sup> and 2'3'-cAMP. These substrates were converted to products by the protein in the crystals itself, showing that the protein is fully functional in the crystalline form. These structures gave

**Beamline I911** is used mainly for macromolecular crystallography (MX) and small-angle X-ray scattering (SAXS), but also other diffraction experiments and for courses. The beamline receives radiation from a superconducting multi-pole wiggler and the wide fan of radiation is shared between five independent branch lines. The central part of the wiggler beam passes through a standard double-crystal monochromator set-up while the four side stations (two on each side) operate at fixed wavelengths. The optics for the side stations consists of horizontally focusing monochromator crystals and vertically focusing curved multilayer mirrors providing fixed wavelength beams. The side stations I911-1 and I911-5 are presently used as test set-ups.

## MX beamlines I911-2 and I911-3

The side station I911-2 (wavelength 1.04 Å) is equipped with a single axis diffractometer and a 165 mm CCD detector. The central beamline I911-3 is tuneable in the range 0.75 – 2.0 Å and is optimized for multiwavelength anomalous diffraction experiments. The beam is vertically collimated by a Rh-coated mirror, monochromatised by a Si(111) double-crystal monochromator and focused by a Rh-coated toroidal mirror. I911-3 is equipped with a microdiffractometer, a mini-kappa, a large-capacity automatic sample changer and a 225 mm CCD detector.

the first detailed information on the reaction mechanism. From comparisons between the structure without a ligand binding and those with the products, flexible loops could be identified that might play a role in substrate recognition. In a follow-up study from this year [3], the use of inactive mutants of CNPase made it possible to obtain the structures of substrate and reaction intermediate analogue complexes, also through data collected at the MX beamlines at MAX II.

In addition, this study also presents, for the first time, a model for the full-length CNPase enzyme. This was achieved by the analysis of small angle X-ray scattering (SAXS) data collected at station I911-4 of the MAX II ring. Together, these studies give a detailed view of the reaction cycle of the enzyme and open up ways to study the specific physiological role of CNPase. This knowledge will lead to an increased understanding of the myelin biology, which is important for the development of new therapies for neurodegenerative diseases, such as MS. ■

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# NOVEL MATERIALS FOR FUEL CELLS

The introduction of fuel cells to the market is limited by the high costs for the platinum electrocatalysts currently used. We have developed and tested a new noble metal-free catalyst concept that consists of metal ions incorporated in a mesoporous carbon matrix. Fuel cell tests using the material show power densities reaching one third of a commercial platinum catalyst. A combination of X-ray absorption spectroscopy and high resolution transmission electron microscopy is used to investigate and understand the chemical state and coordination of the transition metal ions in the new catalysts.

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b. UNIST Central Research Facilities (UCRF) and School of Mechanical & Advanced Materials Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Republic of Korea

c. Graduate School of EWS, WCU Project, KAIST, Daejeon, Republic of Korea

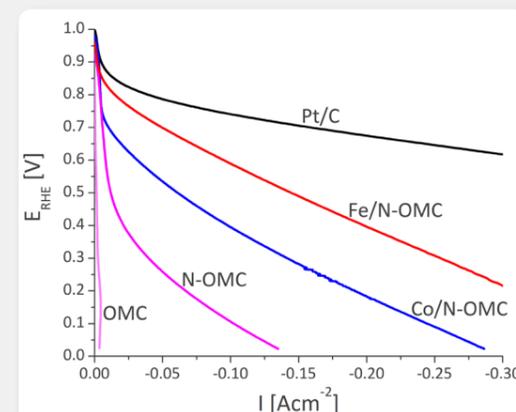
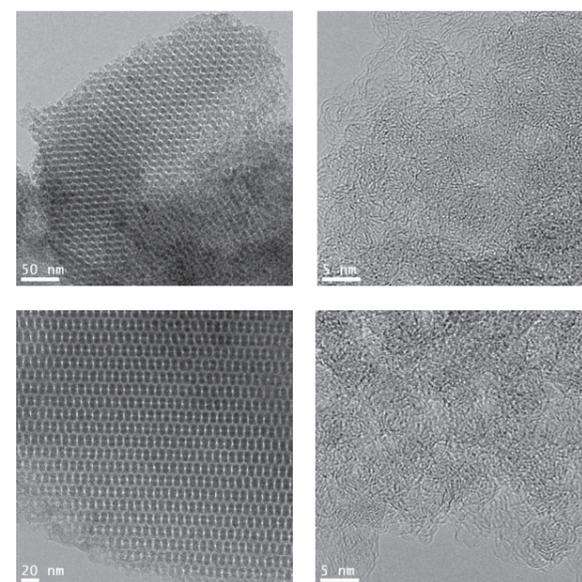
Alternative electrocatalysts for fuel cells should consist of abundant elements, exhibit sufficient activity, stability and efficient mass transport properties. To reach the necessary volumetric activity of the catalyst layer it is necessary to utilize highly porous materials with high specific surface area. In this context ordered mesoporous carbon (OMC) is of great interest as support for electrocatalysts.

Typical OMC materials can reach specific surface areas above 1000 m<sup>2</sup>/g and their mesoscopic pore structure can be fine-tuned in terms of pore size, pore volume, pore wall thickness, atomic as well as mesoscopic structure and degree of hydrophilicity.

In our new catalyst concept we combine the electrocatalytically active local structure of chelated transition metal ions with a high surface area OMC [1]. Through the use of X-ray absorption spectroscopy (XAS) and high resolution transmission electron microscopy (HRTEM) we show unambiguously that the transition metal ions are chelated to the nitrogen-functionalized carbon and not present as metallic, oxide or carbide particles. The transmission electron microscopy images shown in Figure 1 illustrate very high degrees of mesoorder and presence of graphitized carbon layers in catalysts containing either cobalt or iron ions chelated to ordered mesoporous carbons.

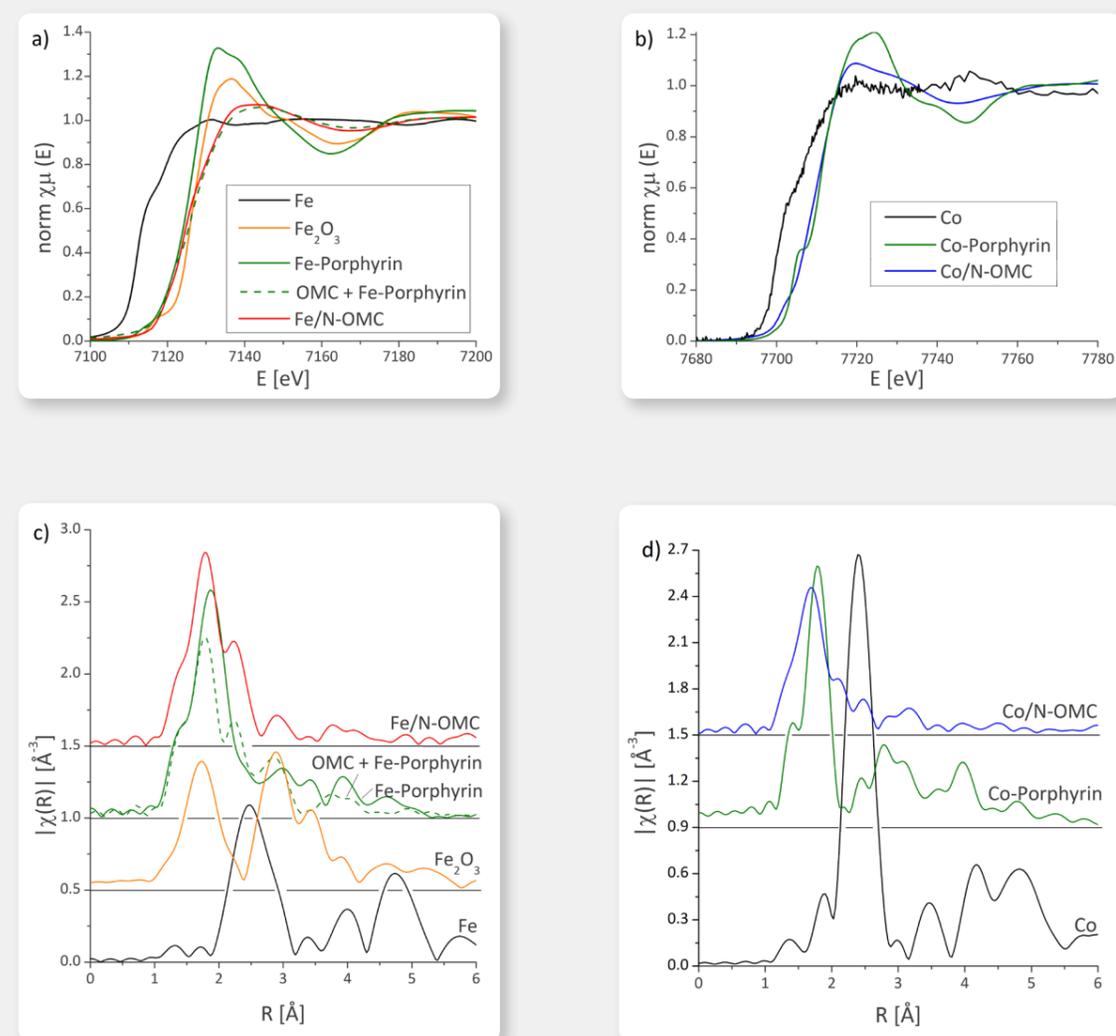
The prepared catalysts are active as cathodes in polymer electrolyte membrane fuel cells. Figure 2 shows the polarization curves of the catalysts compared to a commercial carbon-supported platinum cathode (Pt/C). For comparison, the performance of OMC catalysts without transition metals are shown. Whereas the pure OMC shows no catalytic activity for the reaction within the potential range studied, the nitrogen-functionalized OMC catalyst (N-OMC) shows some activity at potentials below 0.6 V. Introducing transition metals to the nitrogen-functionalized OMC significantly improves the catalytic activity for both cobalt-

**Figure 1.** Transmission electron microscopy images of a cobalt- and nitrogen-functionalized ordered mesoporous carbon (top), and an iron- and nitrogen-functionalized ordered mesoporous carbon (bottom).



**Figure 2.** Single cell fuel cell measurements showing polarization plots for membrane electrode assemblies (MEAs) made from commercial Pt/C anodes and cathodes consisting of ordered mesoporous carbon (OMC), nitrogen-functionalized OMC, and cobalt- or iron-functionalized OMC. A MEA with a commercial Pt/C cathode catalyst is shown for comparison.

**Figure 3.** Iron (a) and cobalt (b) K-edge XAS and radial distance distribution functions (c-d) of functionalized OMCs compared to porphyrins, oxide and metallic samples.



Figures adapted with permission from (Transition Metal Ion-Chelating Ordered Mesoporous Carbons as Noble Metal-Free Fuel Cell Catalysts, Johanna K. Dombrovskis, Hu Y. Jeong, Kjell Fossum, Osamu Terasaki, and Anders E. C. Palmqvist, Chemistry of Materials 25, 856-861 (2013).

and iron-containing catalysts (Co/N-OMC and Fe/N-OMC). The highest activity is found for a Fe/N-OMC with a current density at 0.6 V close to one third of that obtained using the commercial Pt/C cathode in the same measurement setup.

To understand the nature of the catalytically active sites in these catalysts it is relevant to characterize the chemical state and coordination of the transition metals within them. Using HRTEM we do not find metallic or metal oxide particles in the catalysts. Instead, the iron and cobalt present are found to be evenly distributed throughout the materials and possibly atomically dispersed as shown by elemental mapping. The oxidation state and local structure of the transition metals incorporated in the functionalized OMC catalysts can be determined using Fe and Co K-edge XAS, respectively as shown in Figure 3.

From the white line intensities of the normalized absorption plots and from the position of the absorption edge energy of the materials shown it is obvious that the iron and cobalt in the catalysts are present in oxidized states, more similar to that in iron- and cobalt porphyrins than in metallic form. The radial distance distribution plots of

iron and cobalt in the catalysts show unambiguously that the local structure of the metal ions is different from that in metals or oxides and instead more similar to that in the porphyrins and very similar to an OMC impregnated by a porphyrin followed by pyrolysis.

#### Acknowledgements:

The Swedish Research Council (VR) is gratefully acknowledged for project funding and a Senior Researcher grant for AECF. The Swedish Foundation for Internationalization of Research (STINT) is acknowledged for support of a Swedish/Korean research network. TEM work was supported by the year of 2012 Research Fund of the UNIST. Support from the WCU programme, Korea (R-31-2008-000-10055-0) is also acknowledged (O.T.). ■

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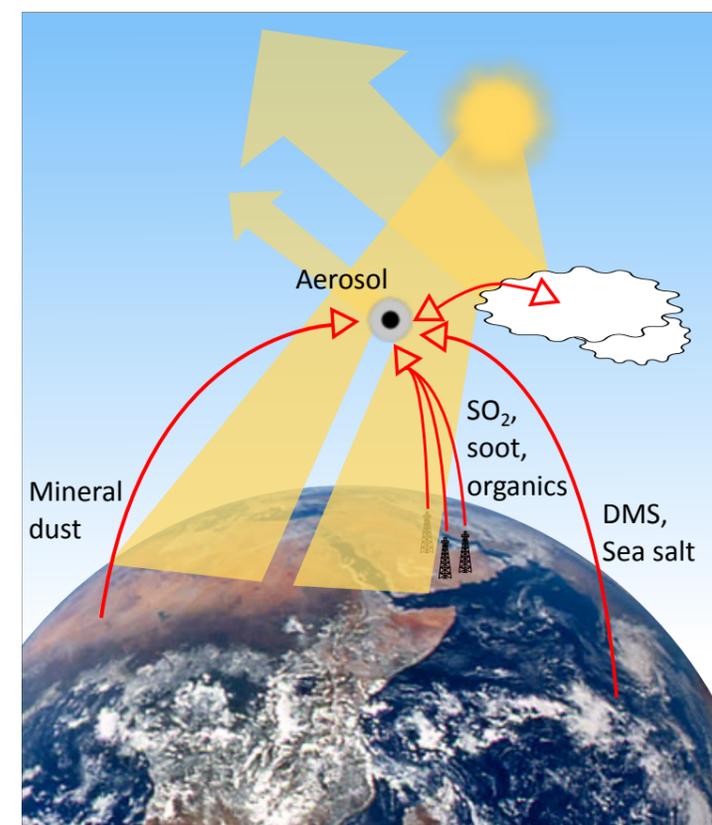
# EXPLORING ATMOSPHERIC AEROSOLS OF CLIMATE RELEVANCE

The atmospheric aerosols influence on cloud formation is the largest uncertainty in climate models. Due to their small size, the surface is important for aerosols. We study how the chemical composition differs between surface and bulk, with the aim to improve representations of aerosol effects in climate models.

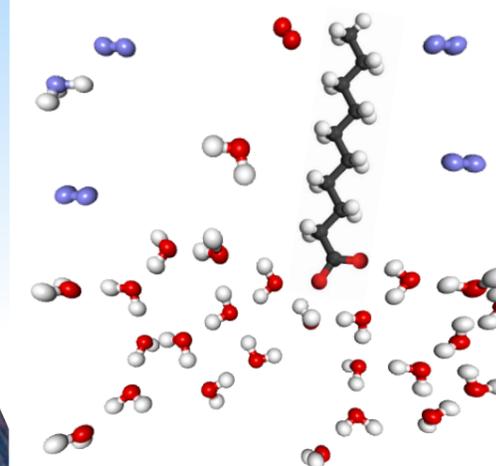
Aerosols are important for atmospheric and climate issues. As illustrated in Figure 1, they affect the global radiative balance, directly by scattering of sunlight and thus increasing Earth's albedo, and indirectly by serving as condensation nuclei for the formation of clouds. It is estimated that the overall effect of the aerosols is to counteract the green house effect by  $\approx 1/3$ , but their effect has been identified by the Intergovernmental Panel on Climate Change (IPCC) as a key uncertainty in predicting climate change [1].

In the atmosphere there are species of both biogenic and anthropogenic origin incorporated into aqueous aerosols. This includes salt ions from the sea, organic molecules from forests, soot from combustion, pollutants and mineral particles. These aerosols are secondarily influenced by ionizing radiation and chemical reactions, resulting in a broad range of complex compositions. An example of this is hydrocarbons from e.g. forests and fossil fuel combustion, oxidized into carboxylic acids, which are important compounds in so called Secondary Organic Aerosols (SOA) [2].

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 a. Department of Physics, University of Helsinki, Helsinki, Finland  
 b. Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden  
 c. MAX IV Laboratory, Lund University, Lund, Sweden



**Figure 1.** Aerosols are microscopic particles, which are either emitted directly into the atmosphere or formed there. They cool the earth directly by reflecting incoming sunlight, and indirectly by regulating cloud formation. Due to their small size, the aerosol surface is very important for their macroscopic properties, and we study its microscopic composition. Image of Earth courtesy of the Image Science & Analysis Laboratory, NASA Johnson Space Center.



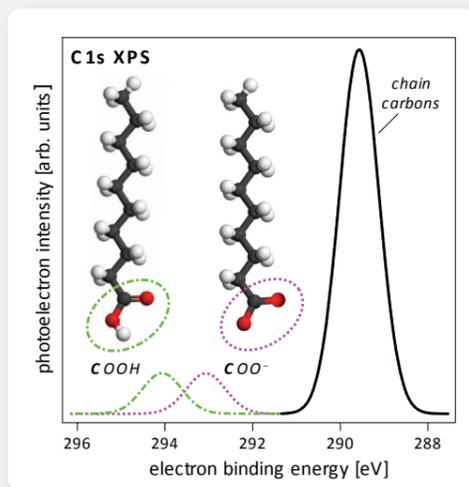
Stefan Carlson  
Beamline scientist I811

PhD in chemistry,  
Stockholm University  
At MAX IV Laboratory since 2001

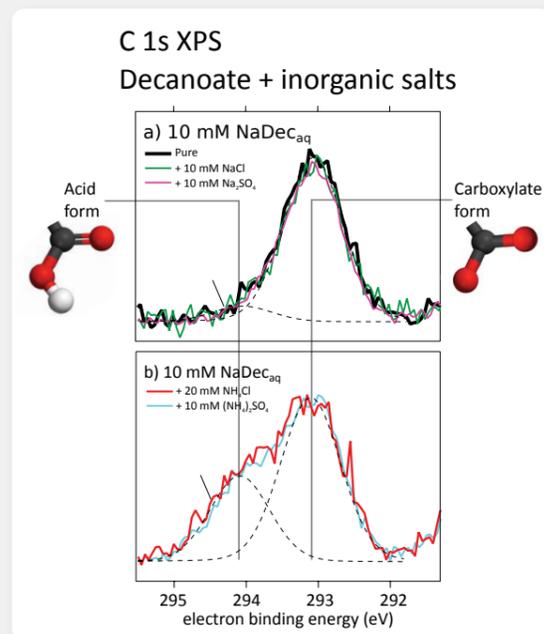
The XAS user community at beam line I811 studies a wide range of topics; materials, environmental, physics and chemistry, and also life sciences. Catalysis research is the big thing at the moment.

Making in-situ analyses on catalyst materials during the reaction gives the users direct information on how the materials behave. In this respect, I811 has an important role in the search for new and better catalytic materials.

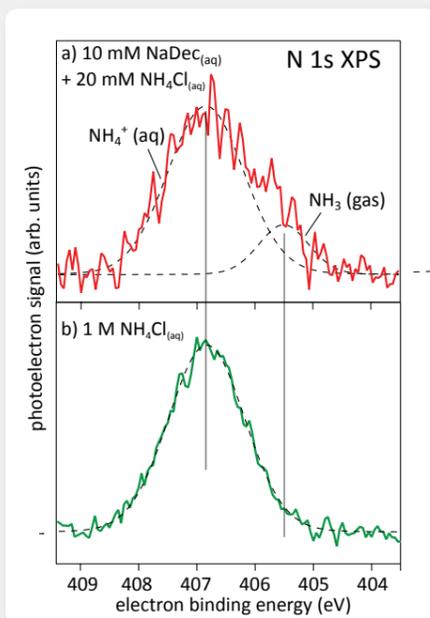
Beamline I811 is used for X-ray absorption spectroscopy (EXAFS and XANES) and X-ray diffraction (XRD) experiments. It is based on a super-conducting multipole wiggler insertion device that produces high-flux photons in the energy range 2.4 - 20 keV (0.6-5 Å). The design is based on adaptive optics where the beam is collimated and focused vertically by cylindrical bendable first and second mirrors, respectively. Horizontal focusing is obtained by sagittal bending of the second monochromator crystal. The typical flux in a 1 x 1 mm<sup>2</sup> beam spot on the sample is 5·10<sup>11</sup> photons/sec. One experimental station is used for XAS research with detectors for transmission and fluorescence yield techniques. A second station is equipped with a diffractometer for surface, interface and thin-film crystallography.



**Figure 2.** A schematic C1s XPS spectrum for Dec- and DecH, demonstrating how the signal from the carboxylate/carboxylic carbon can be used to distinguish between the Dec- and DecH species.



**Figure 3.** C1s XPS spectra of NaDec together with the salts NaCl and Na<sub>2</sub>SO<sub>4</sub> (top), and NH<sub>4</sub>Cl and (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> (bottom), demonstrating that the NH<sub>4</sub><sup>+</sup> ions are responsible for the conversion of Dec- to DecH on the surface.



**Figure 4.** N1s XPS spectra of the salt NH<sub>4</sub>Cl in solution (bottom) and NH<sub>4</sub>Cl + NaDec in solution (top), demonstrating the formation of gaseous NH<sub>3</sub> from NH<sub>4</sub><sup>+</sup> ions at the surface.

Even though only ≈0.01% of all water on Earth can be found in the atmosphere, the total air-water interface area of this small fraction is larger than that of all the oceans together due to the small size of the atmospheric water particles. The microscopic size of aerosols makes the surface important for their properties and atmospheric influence. The surface composition may be different from the bulk due to surface segregation effects. This affects e.g. surface tension, which in its turn affects if and how aerosol particles grow into droplets, and thereby macroscopic cloud properties such as reflectivity. A differing surface composition is also important for atmospheric chemistry, as species at the surface are more exposed to radicals. We study aqueous surfaces using X-ray photoelectron spectroscopy (XPS), a technique that is both chemically sensitive and surface sensitive, at the I411 beamline at MAX-lab [3].

We have studied the surface speciation of decanoate (Dec-). Dec- is the de-protonated form of the typical fatty acid decanoic acid (DecH), formed by oxidation of organic material. Due its long hydrophobic aliphatic chain, the Dec- ions are surface active, i.e. enriched at the surface.

To illustrate the chemical sensitivity of XPS, an idealized spectrum for an aqueous mixture of Dec- and DecH is

shown in Figure 2. The three peaks correspond to C1s electrons originating from the chemically inequivalent aliphatic (methyl and methylene), carboxylate, and carboxylic carbons, respectively. We primarily focus on the C1s signal from the carboxylate/carboxylic group, as this is a sensitive fingerprint of the protonation degree.

Aerosols often contain inorganic salts, such as NaCl and (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>. One common effect of inorganic salts on solvated organic ions or molecules is “salting out”, i.e. the increase of the organic ions or molecules at the surface due to competition for solvating water molecules. We investigated the effect of NaCl and (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> on aqueous NaDec, see the green and blue spectra in Figure 3 [4]. In the low concentrations investigated, the salting out effects of both salts are relatively weak, but surprisingly (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> has an additional effect; the protonated form DecH is formed. By instead adding the salts NH<sub>4</sub>Cl and Na<sub>2</sub>SO<sub>4</sub>, we see that DecH is also formed by NH<sub>4</sub>Cl but not by Na<sub>2</sub>SO<sub>4</sub> (red and pink spectra in Figure 3, respectively) [4]. This means that it is the ammonium ions NH<sub>4</sub><sup>+</sup> that are involved in the conversion of Dec- into DecH: Dec- + NH<sub>4</sub><sup>+</sup> → DecH + NH<sub>3</sub> (possibly mediated through neighbouring water molecules). This is a surface-specific reaction that does not occur in bulk solution. In other words: The overall composition of the aqueous phase is not changed much, even when the surface properties undergo significant changes! Another aspect of

this process is that some of the NH<sub>3</sub> which is formed at the aqueous surface leaves the solution, as evidenced by the gaseous NH<sub>3</sub> signal seen in the N1s XPS spectra of NaDec + NH<sub>4</sub>Cl (Figure 4) [4].

These findings demonstrate that the chemical composition of the aqueous surface may differ from that of the bulk and may change dramatically without corresponding changes simultaneously occurring in the bulk phase. Our research now continues in two directions: to quantify the surface-specific reaction and to survey the surface propensity of organics connected to SOA as function of factors such as concentration, salt co-solvation and pH, aiming at quantifying and parameterizing the results so that they can be included in, and thereby improving, climate models. ■

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At MAX IV Laboratory since 2000

**At the I411 users** mainly look at different systems in gas phase, it can be atoms or molecules, or it can be a beam of particles or a beam of liquids. Users look at different properties depending on the system. In the article, for example, one looks at how ions distribute themselves in a liquid.

**Beamline I411** is based on an SX-700 type PGM and an undulator source (43-period, 59 mm period length) that covers the photon energy range 40 eV to about 1500 eV. The end-station has the unique versatility of being able to handle solid, liquid and gaseous samples. Thus the beamline is well suited for high-resolution electron spectroscopy on free atoms and molecules as well as for studies of liquids and non-UHV compatible solids.

The experimental system consists of separate analyser and preparation chambers accessible via a long-travel manipulator. The analyser chamber is equipped with a hemispherical electron energy analyser (SCIENTA R4000) which can be rotated around the incoming beam for polarization dependent measurements. In front of the experimental station a one-meter long section of the beamline can host other types of equipment for atomic and molecular spectroscopy, e.g. ion-electron coincidence detectors. A laser system for two-colour experiments is also available.

# THE VALLEY DEGREE OF FREEDOM IN A 2D SPIN-POLARIZED ELECTRONIC SYSTEM

Exotic physical phenomena arise when a little more than one atomic layer of Thallium is grown on silicon. Synchrotron radiation is used to investigate this interesting system which shows promising applications in spintronics; electronics using electron's spin states in addition to its charge.

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The decrease in size of a crystal to nanometre scale leads to a reduction from a three-dimensional to a lower dimensional periodical structure and is often accompanied with the appearance of novel exotic solid-state properties. In the case of a reduction into a two-dimensional (2D) system, a spin-polarised 2D electronic structure is formed by spin-orbit coupling in combination with space inversion asymmetry even for nonmagnetic materials. This so-called Rashba-Bychkov (RB) effect ordinarily produces a pair of spin-polarised bands in  $k$  space with the spin polarisation vector in the surface plane and a Fermi surface consisting of two concentric circles with opposite chiral spin textures as shown in Figure 1.

The application of the RB effect in spintronics (devices using spin degree of freedom in addition to the charge degree of freedom) was first proposed 20 years ago and is still unrealised to date. The main problems stems from the presence of the two Fermi circles and the low spin polarisation, both of which allow electrons to backscatter (Figure 1a) and thus greatly reduce the efficiency of the spin transport. A very promising approach is to use the valley degrees of freedom to restrict the scattering directions (Figure 1b) and then to 100 % spin-polarise the valleys to suppress the probability of backscattering (Figure 1c).

In order to accomplish this project, an international team led by the Chiba group performed high-resolution angle-resolved photoelectron spectroscopy (ARPES) measurements at the I4 beamline at MAX-lab, as well as other measurements such as spin-resolved ARPES and scanning tunneling microscopy/spectroscopy at different facilities. The system used in the project is a Si(111) surface with slightly more than one monolayer (ML) of Tl on top. The advantage of using Si as a substrate is to pave way towards the realisation of silicon spintronic devices. The heavy element Tl with strong spin-orbit coupling induces the large spin splitting that is responsible for the spin-polarised valleys. The 1 ML Tl atoms adsorb on the three-fold hollow site (the  $T_4$  site) of the Si(111) ideal surface forming a three fold symmetric structure with mirror planes in the  $[11\bar{2}]$  and the two other corresponding directions (Figure 2a). The  $C_3$  symmetry (Figure 2b), of the system lifts the spin degeneracy forcing the spin to be fully polarised with the polarisation vector perpendicular to the surface (Figure 3a). The degree of polarisation and the direction of the spin are different from those of normal Rashba systems (Figure 1a). However, these states are at binding energies of approximately 1.5-2.0 eV below the Fermi level and will therefore hardly contribute to spin transport.

The addition of a small amount of extra Tl, electron-dopes the system and a state appears at the Fermi level with an extra Tl coverage of 0.01 ML, and it moves continuously downward in energy by adding more Tl (Figure 3b). These extra Tl atoms are adsorbed on the three-fold hollow site of Tl/Si(111)-(1x1) and does not change the underneath  $C_3$  symmetry between 1.00 and 1.12 ML. The inversion asymmetry lifts the spin degeneracy and the preservation of time-reversal symmetry [ $E(\mathbf{k},\uparrow) = E(-\mathbf{k},\downarrow)$ ] lead to opposite spin directions at  $\bar{K}$  and  $\bar{K}'$ . These metallic bands are 100% spin-polarised along the surface normal direction with opposite polarisation vectors at  $\bar{K}$  and  $\bar{K}'$ . Furthermore, the same effective mass along the  $k_x$  and  $k_y$  direction and the roughly circular shape of the Fermi surface indicate that these spin-polarised metallic band form "valleys" with a parabolic shape at the  $\bar{K}$  and  $\bar{K}'$  points (Figure 3c). The Fermi surface and its spin structure govern the elastic electron scattering between states located in a single valley (intravalley scattering), and states located in two valleys at  $\bar{K}$  ( $\bar{K}'$ ) points (intervalley scattering). At the bottom of the valley, the spin polarisation vector remains unchanged indicating that the backscattering can be tuned to disappear in the diametrically opposite direction. This is in contrast to normal Rashba systems with spin polarisation parallel to the surface, where the backscattering would be possible even at the bottom of the

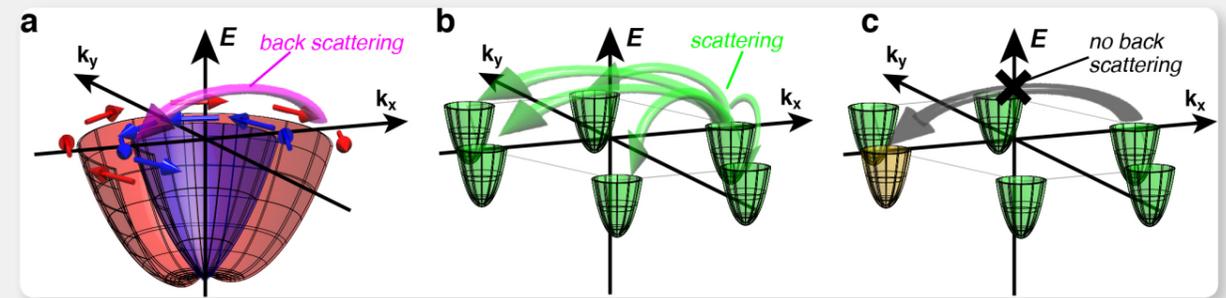


Figure 1. Spin-polarised bands of (a) an ordinary Rashba system, where the scattering may occur in any direction, and (b) a system with non-polarised electron valleys at the  $\bar{K}$  and  $\bar{K}'$  points of the SBZ, where scattering is limited to the  $\bar{K}$ - $\bar{K}'$  directions. (c) A system in which one valley is polarised, and thus electrons cannot backscatter.

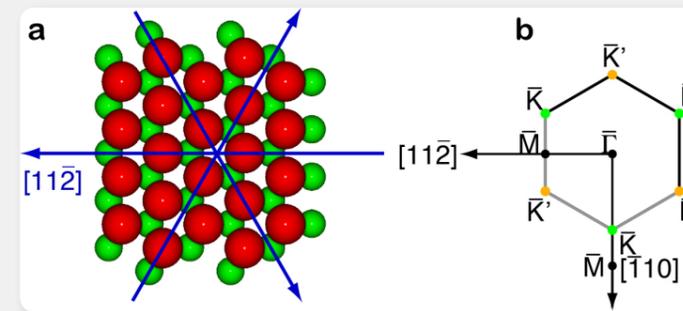


Figure 2. (a) Atomic structure of the system used in the present project. Red and green circles represent the Tl and Si atoms, and the blue arrows indicate the mirror planes. (b) The surface Brillouin zone of Tl/Si(111) where  $\bar{K}$  and  $\bar{K}'$  are indicated by green and orange circles.

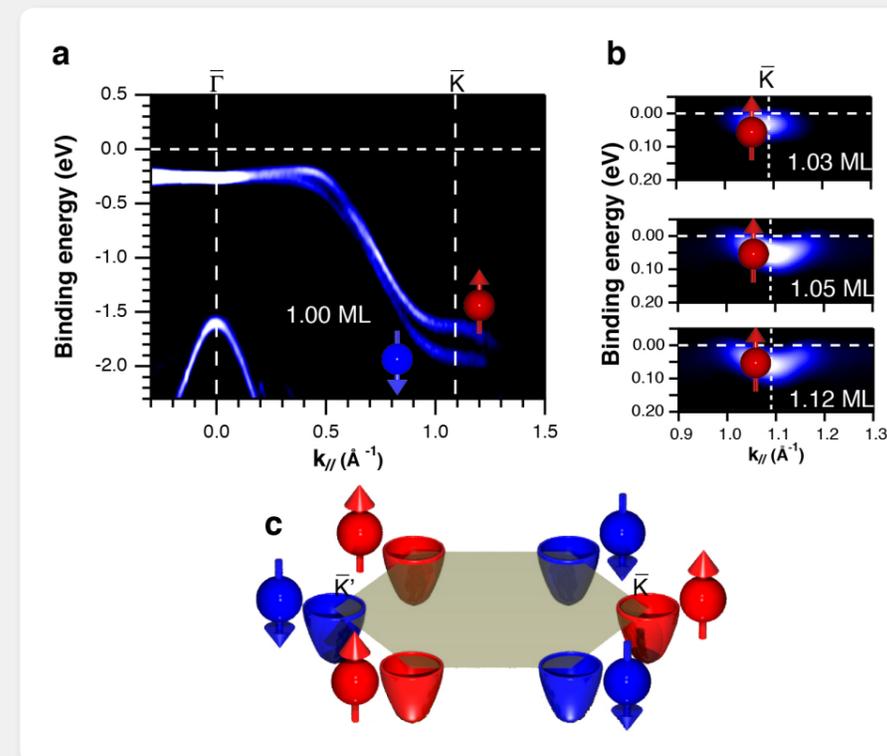


Figure 3. (a) ARPES result of a Si(111) surface covered with 1.00 ML of Tl. (b) Metallic band observed at the  $\bar{K}$  point for different Tl coverage. (c) Schematic illustration of the spin-polarised surface states at  $\bar{K}$  and  $\bar{K}'$ . The gray hexagon represents the SBZ, and the position of the SBZ is here used to indicate the Fermi level at coverage of 1.12 ML.

valley. The results obtained in this project show that it is possible to completely spin-polarise the valleys in an easy and simple way and make them act as filters that suppress the backscattering of spin carriers by considering the symmetry of the surface. This method of polarising the valleys is much simpler than the methods proposed previously to polarise the valleys of graphene. It also shows that combining peculiar Rashba spins with valleytronics opens up an avenue to greatly improve the efficiency of spin currents for silicon spintronics applications.

#### Acknowledgements:

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**Basic science** is the main theme at this beamline, which is used for angle resolved photoelectron spectroscopy on solids.

**Users study electron structure** in different solid materials to understand their electronic properties. Graphene, the topic of the Nobel prize in physics 2010, has been studied at this beamline.

**Topological insulators** are the hottest materials at present, they present fundamentally new physics in addition to holding promise for spintronics applications.

**Beamline I4** is an undulator beamline used for angle resolved photoemission. It is equipped with a spherical grating monochromator covering the energy range 13 to 200 eV.

The end station analyser chamber hosts two electron energy analysers: An in vacuum rotatable VG ARUPS 10 analyser and a fixed mounted PHOIBOS 100 mm CCD analyser from SPECS. The SPECS analyser has an ultimate resolution of less than 3 meV. There are three angular dispersion modes namely MAD (medium angular dispersion), LAD (low angular dispersion) and WAM (wide angular dispersion). The MAD mode has angular acceptance of  $\pm 3$  degrees with angular resolution of less than 0.1 degrees. The LAD mode has angular acceptance of  $\pm 6$  degrees with angular resolution of about 0.15 degrees. The WAM mode has angular acceptance of  $\pm 10.5$  degrees with angular resolution of about 0.4 degrees.

# ORIENTATIONAL ORDER IN A COLLOIDAL GLASS

Glasses are fascinating materials with slow dynamics and an amorphous structure. Their history dependence means that sample handling can profoundly affect physical properties. Here we investigate how solvent evaporation from a colloidal glass of clay platelets can induce orientational order, leading to an optically anisotropic colloidal glass.

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Colloidal glasses are a fascinating class of soft solids. They are formed when dispersions of small nano- to micro-sized particles become crowded so that the dynamics of the particles slow down, although the interparticle structure remains amorphous. For slightly polydisperse hard sphere colloids, a glassy system can then form at particle volume fractions between roughly 0.58 and 0.64, the latter being the volume fraction for random close packing of a monodisperse system [1].

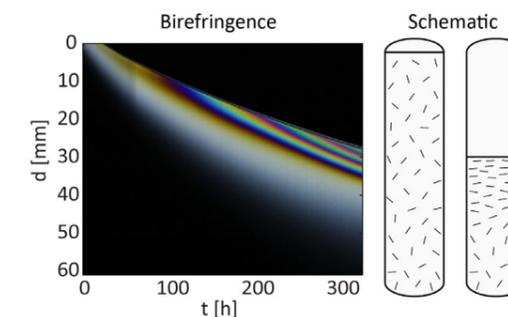
This situation changes when particles are non-spherical and carry electrostatic charges, as is the case for clay platelets dispersed in water. Glassy dynamics can then occur at much lower volume fractions and may involve not only the translational movements of the particles, but also rotational motions. Such systems may form orientational glasses (with slow rotations) [2-4], 'simple' glasses (with slow translations) [5], or double glasses (with slow rotations and translations) [4-7], as well as equilibrium phases like nematic liquid crystals [8-11].

When glassy systems form, their physical properties become dependent upon their history. This is a hallmark of an out-of-equilibrium system, which will undergo aging as it evolves towards equilibrium, albeit slowly [1]. The history dependence of glasses means that sample handling can significantly affect sample properties.

Here we use 3.0 wt% dispersions of Laponite (LRD) in deionized water to show that orientational order can develop in glassy dispersions of charged platelets when a concentration gradient is imposed through solvent evaporation [12]. In deionized water, Laponite exists as slightly less than 1 nm thick disc-like particles with diameters of approximately 25 nm. The particles carry a net negative surface charge. At a concentration of 3.0 wt% in deionized water, Laponite is reported to form orientationally dis-

ordered glasses whose translational as well as rotational dynamics slow down with time [7, 12-18]. Small-angle X-ray scattering (SAXS) experiments on such non-evaporated samples give isotropic scattering patterns indicating no net orientational order and only short-range positional order, expected from crowding [12].

A different behavior occurs when samples are allowed to undergo slow evaporation. A spatio-temporal plot of an evaporating sample (Figure 1) shows birefringence,  $\Delta n$ , that grows from the evaporation interface towards the bulk, invading the sample on macroscopic length scales on the order of centimetres in a matter of weeks. Because the birefringence remains unchanged when samples are rotated by an angle  $\theta$  around their cylinder axis, the ordering must constitute a cylindrically symmetric distribution of particle normals around this axis. The successive changes of the birefringence colours (determined by the retardation  $\Delta n \cdot l$ , with  $l$  the sample thickness) signals the existence of a long-



**Figure 1.** Birefringence image of the spatio-temporal evolution of a Laponite glass during water evaporation. Each column of pixels shows the central part of the sample photographed at increasing waiting times. The sample thickness was  $l=2.65$  mm. The schematic illustrates the deduced structure of the sample at the beginning and the end of the evaporation process respectively.

lived gradient in either the order (as characterized e.g. via the nematic order parameter  $S_2$ ), in the concentration of particles (or equivalently the volume fraction  $\Phi$ ), or both (because  $\Delta n \sim S_2 \Phi$ ) [19].

We confirm the presence of a gradient in  $\Phi$  using the X-ray transmission. From this analysis, volume fractions around  $\Phi=2\%$  are obtained in non-evaporated samples or in evaporated ones far away from the interface, whereas close to the interface the volume fraction gradually rises, reaching above  $\Phi=6\%$  in some cases [12]. By converting volume fraction data to particle concentrations, we find that the concentration near the interface exceeds 9 wt%, reaching well into the range where experimental studies have observed textures reminiscent of nematic defects in Laponite dispersions [20], but where simulations yield arrested dynamics without order [21].

From the SAXS data we find that a gradient in the order parameter  $S_2$  exists alongside the volume fraction gradient [12]. We obtain a quantitative measure of the order by comparing the anisotropy of the SAXS data (in the q-range where the structure factor is flat), to simulated SAXS patterns computed with a suitable orientational distribution [12]. From this analysis, we prove that even our most anisotropic SAXS patterns (Figure 2) correspond to relatively low values of the order parameter ( $S_2 \leq 0.21$ ). We also find that the relationship between  $S_2$  and  $\Phi$  appears relatively well-defined within the uncertainty associated with our measurements, and that this relationship reproduces across the investigated samples [12].

The origin of orientational order in Laponite dispersions has been an unresolved issue [22]. Early observations found that viscoelastic samples could display textures reminiscent of nematic defects [20]. Later on, a study of oedometrically compressed samples with NMR [23] found orientational order developing with the concentration in a similar manner to that found in our samples, albeit at higher salt concentrations. The compression study however predicts perfect order at very high volume fractions. This is similar to what is predicted by our  $S_2$  versus  $\Phi$  data, where an order parameter of  $S_2=1$  (perfect orientational order) is achieved only when  $\Phi=90\%$  [12].

Well before such high volume fractions are reached, we note that samples are prone to fracture, pointing to the evaporation process causing significant stresses on the glass. We estimate that the evaporation-induced compression of the colloidal structure causes an average normal rate of deformation two orders of magnitude larger than the inverse of the estimated structural relaxation time,

obtained from dynamic light scattering (DLS) [12]. This implies that the response of our samples to such strain rates is solid-like, i.e. is elastic or plastic.

Plastic events, which involve irreversible displacements or reorientations, are known to impart permanent anisotropies to e.g. simulated, sheared silica glasses [24]. However, although such plastic events drive the system from less to more favoured configurations under stress, it is important to note that the order resulting from deformations is generally not intrinsic but history-dependent.

We therefore conclude that the birefringence in our samples is due to plastic deformations driving the initially disordered glass into a state where a long-lived concentration gradient is accompanied by orientational particle ordering. This process may be used to create a colloidal glass with a well-defined gradient in optical properties. ■

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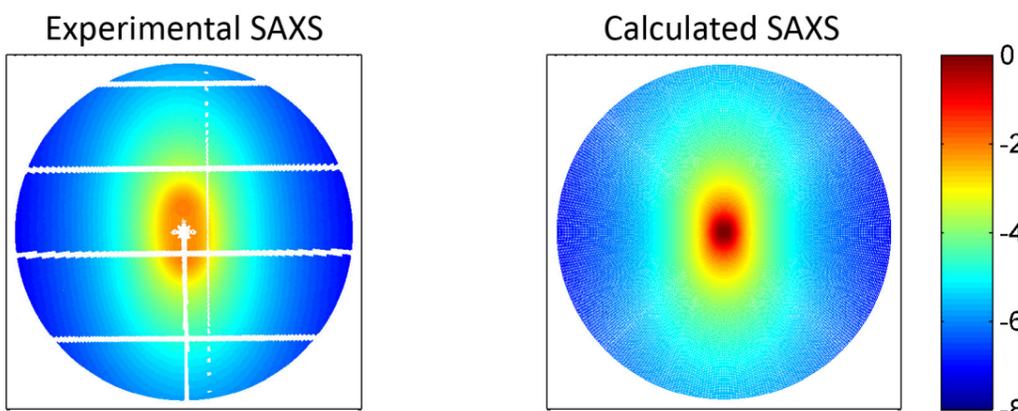
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The SAXS user community comes from diverse fields of research with different needs and requirements at the end-station but with one common goal: understanding complex nanostructured materials. At I911-SAXS measurements of biological macromolecules and membranes in solutions, natural and synthetic polymers, amorphous and crystalline materials in different states like solids, liquids, gels or powders and gases have been performed. Synchrotron SAXS is a powerful, non-destructive technique which can provide information in small volume sizes (lower than 0.1 mm<sup>3</sup>) and in seconds time resolution.

#### SAXS beamline I911-4

The new SAXS station, I911-4, has a fixed wavelength beam (0.91 Å) and is equipped with a two dimensional Pilatus 1M detector (*Dectris*). The accessible q-range is typically 0.008 – 0.4 Å<sup>-1</sup> but it can be extended by changing the set-up to 0.006 or 2 Å<sup>-1</sup>. The beamline offers dedicated set-ups for high throughput solution scattering and combined spectroscopy / X-ray scattering techniques. It is also possible to install custom made set-ups provided by the users, for example ultrasonic levitators, tensile test devices, high temperature systems and syringe pump flow cells.

**Figure 2.** Measured and calculated small-angle X-ray scattering patterns. The measured pattern was recorded near the interface of a sample following evaporation. The calculated pattern originates from a distribution of particle normals with an order parameter of  $S_2=0.21$ . The intensity scale is logarithmic and normalized. The q-range is  $0.06 \text{ nm}^{-1} \leq q \leq 2.6 \text{ nm}^{-1}$  in the experimental data and  $0.003 \text{ nm}^{-1} \leq q \leq 2.6 \text{ nm}^{-1}$  in the calculated pattern.



# ULTRAFAST CHARGE TRANSFER IN DYE-SENSITIZED SOLAR CELLS

Dye-sensitized solar cells (DSCs) offer a promising cheaper alternative to conventional silicon based solar cells. In this study [1] resonant inelastic X-ray scattering (RIXS) has been used to reveal ultrafast charge transfer (CT) occurring in only 2.8 femtoseconds from dye molecules to the conduction band of the TiO<sub>2</sub> substrate in a DSC.

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DSCs operate using thin photosensitive dye films, most commonly a ruthenium-based dye adsorbed onto the surfaces of interconnected titanium dioxide colloidal nanoparticles (Figure 1). Incoming photons excite electrons in the dye molecules, which are then transferred to the TiO<sub>2</sub> conduction band and finally to the anode of the cell thus creating an electrical current. Understanding the dynamics of CT from the molecule to the substrate is a key step to understanding dye-sensitized solar cells.

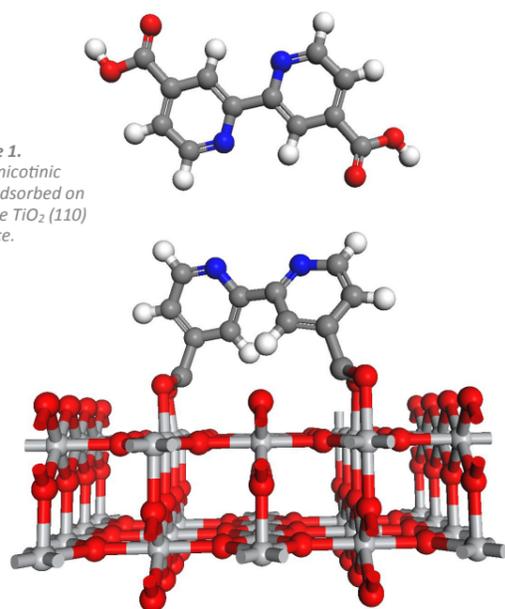


Figure 1. Bi-isonicotinic acid adsorbed on a rutile TiO<sub>2</sub> (110) surface.

CT has to be fast enough to compete against loss processes to achieve high efficiencies and avoid photodegradation of the dye molecules. Core-level spectroscopic techniques such as RIXS are well suited for studies of these dynamics. RIXS is a photon-in, photon-out based technique, which means that the sample environment can be separated from the vacuum needed to conduct the experiments allowing studies of vacuum incompatible samples. It is also bulk sensitive allowing you to probe deeper into the sample than competing techniques. This opens up for future possibilities to extend the technique to real-life samples, and not limited to prototype samples prepared to be vacuum compatible.

In RIXS the energy of the impinging photon is tuned to a resonance corresponding to exciting one of the core electrons of an atom to one of the unoccupied orbitals in the molecule that the atom belongs to, for example the Lowest Unoccupied Molecular Orbital (LUMO). The photon will then undergo either elastic scattering or inelastic scattering. The first will give rise to a so called participator decay feature in the resulting X-ray emission spectra, corresponding to the excited electron decaying back to fill the core-hole. The latter is called spectator decay and comes from the core-hole being filled by one of the valence electrons, giving a valence excited final state to the scattering. Note that both processes will leave the molecule in a non-ionized final state. The RIXS process is illustrated in Figure 2.

CT will be seen as a change in the resonant behavior of the participator decay channel. If CT is happening on a time-scale comparable to the core-hole lifetime we should see a weakening of the participator decay peak in the RIXS spectra. For CT to happen the energy of the core-excited molecule must lie above the conduction band of the substrate. If one of the LUMOs of the core-excited molecule lie below the conduction band we can use a concept called the core-hole clock (CHC) [2, 3, 4] well established in resonant photoemission to estimate the CT time. This is possible since it provides us with an intrinsic reference point for normalizing the abundance of participator electrons measured for those states that overlap with the conduction band of the substrate, where CT is possible.

Both a monolayer as well as a multilayer of bi-isonicotinic acid adsorbed on a rutile TiO<sub>2</sub> (110) surface were studied. N1s X-ray absorption spectra for the multilayer and monolayer of bi-isonicotinic acid on the TiO<sub>2</sub> (110) surface are shown in Figure 3. The LUMO resonance of the multilayer occurs at 398.8 eV, and the LUMO+1 resonance, at 400.1 eV. The LUMO resonance of the chemisorbed molecules in the monolayer occurs at a photon energy of 398.6 eV and the LUMO+1, at 400.5 eV. From the alignment of valence photoemission, X-ray absorption and the substrate density

## Resonant Inelastic X-ray Scattering

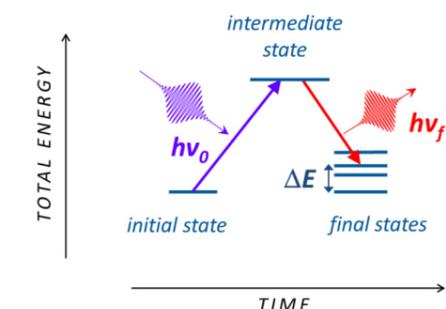
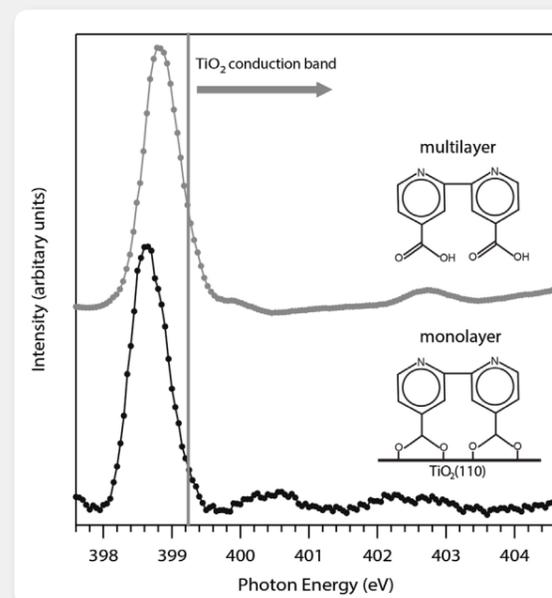


Figure 2. Resonant inelastic X-ray scattering (RIXS). Illustration from [8].

Figure 3. N1s fluorescence yield X-ray absorption spectra for a multilayer and monolayer of bi-isonicotinic acid, on the TiO<sub>2</sub> (110) surface, normalized to the intensity of the LUMO resonance. From Ref [1]. Copyright (2012) by the American Physical Society.



Beamline I511 was used for RIXS, XAS, XPS, and X-ray emission spectroscopy (XES) in the VUV and soft X-ray range. It was decommissioned during 2013 and mounting of the SPECIES beamline has since started. The new SPECIES beamline uses a common EPU and collimated PGM monochromator allowing for direction of the radiation alternately into two experimental stations. The undulator has a 61 mm period length giving a photon energy range of 27 to about 1500 eV.



Conny S the  
Beamline scientist SPECIES

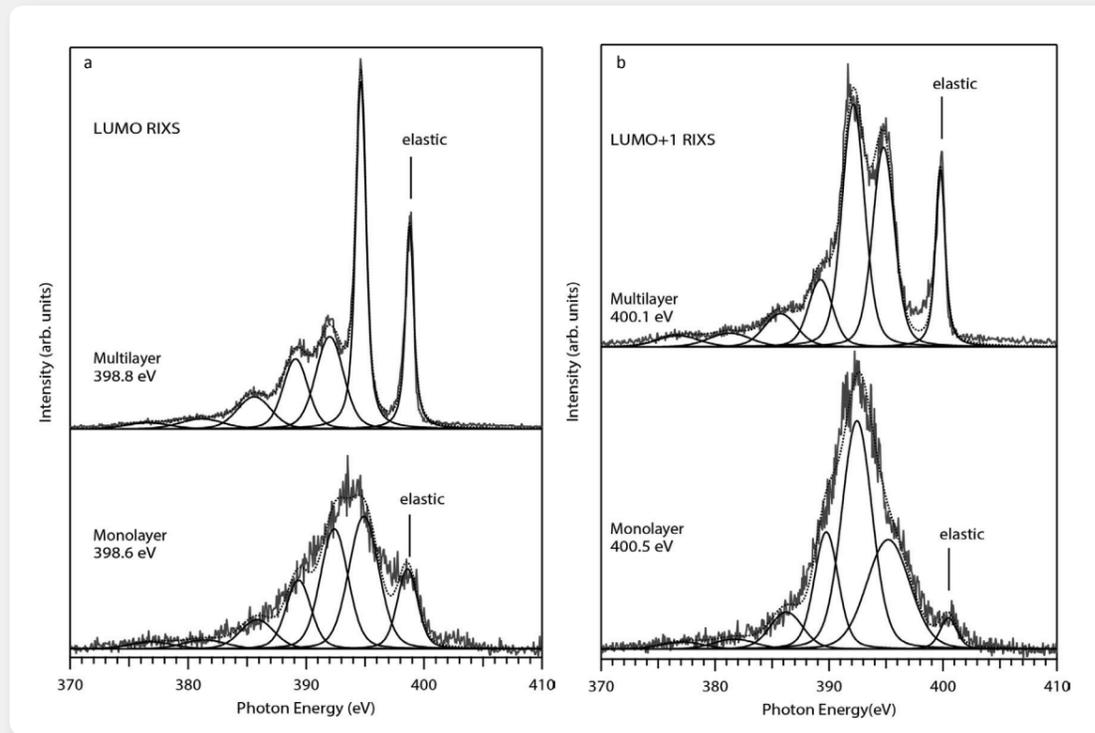
PhD in physics, Uppsala University  
At MAX IV Laboratory since 2012

The I511/SPECIES beamline has two experimental stations focusing on core-electron spectroscopies in the soft X-ray energy region (27-1500 eV).

A broad set of tools are provided by the beamline for the study of electronic structure in molecules, liquids and solids. It features support for ambient pressure sample environments for both photon-in, photon-out techniques and photoemission.

This lets us study samples under real conditions for applications like Li-based batteries, corrosion processes and as in the case of this highlight, dye-sensitized solar cells. Users of the beamline range from such diverse fields as material sciences, catalysis research and biochemistry.

# CURRENT BEAMLINES AT MAX-LAB



**Figure 4.** (a) RIXS spectra, at the LUMO resonance, for both the multilayer (on top) and monolayer (on bottom), of bi-isonicotinic acid, on the rutile  $\text{TiO}_2$  (110) surface. Spectra have been normalized to the total area. (b) RIXS at the LUMO+1 resonance, for both the multilayer (on top) and monolayer (on bottom), of bi-isonicotinic acid, on the rutile  $\text{TiO}_2$  (110) surface. Spectra have been normalized to the total area. From Ref [1]. Copyright (2012) by the American Physical Society.

of states for this system [3, 5, 6], the LUMO state of the monolayer is known to be 0.6 eV below the conduction band of titanium oxide while the multilayer is isolated from the surface in a thick film. It is thus only expected to see CT in the participator decay feature in the RIXS spectra from the LUMO+1 resonance from the monolayer. This was verified by the experiment (Figure 4a and 4b). For a full analysis giving an estimated time for the CT of  $2.8 \pm 1.5$  fs we refer you to the research paper itself [1].

The research was done on the I511 beamline at MAX-lab using a modified Nordgren type [7] grazing incidence spectrometer to record the RIXS spectra. I511 is currently being replaced by the new SPECIES beamline and will feature an upgraded version of the same instrument. This new instrument will take full advantage of the smaller source size, operating in slit-less mode. A new experimental chamber has been

designed to provide better adaptability to different sample environments. Including the availability of a liquid flow cell that could be adapted to the study of real condition DSCs. ■

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There are currently 14 beamlines in operation and one under construction at the three MAX-lab rings. The majority of the beamlines are installed at the MAX II ring, while three beamlines for measurements in the ultraviolet and infrared are installed at the MAX III ring. MAX I is in addition used as a pulse stretcher for nuclear physics experiments. For a detailed description of the beamlines, see the chapter Scientific Highlights and tables 1, 2 and 3 below.

Major achievements during 2013 include the installation and test of the EPU61 undulator at I511, the decommissioning of the I511 beamline and the start of mounting the replacement beamline SPECIES, the finalization of the commissioning of the infrared spectromicroscopy beamline D7 on MAX III, and the installation of a protein solution robotic system at beamline I911-4.

## MAX I Beamlines

MAX I is used as an electron pulse stretcher to create high energy light for nuclear physics reactions.

## MAX II Beamlines

The 1.5 GeV MAX II storage ring is equipped with two planar undulators and two EPU's for the VUV and soft X-ray regions and three multi-pole wigglers for the X-ray region. One conventional multi-pole wiggler beamline is used for powder diffraction. Of the two superconducting multi-pole wigglers, one is used for a materials science beamline for absorption and diffraction experiments (I811) and the other (I911) is used for a system of five independent beamlines, mainly for protein crystallography and small angle X-ray scattering. The undulators serve beamlines with a variety of spectroscopic techniques such as X-ray absorption (including circular dichroism), X-ray emission, X-ray photoelectron

spectroscopy and photoemission electron microscopy in the VUV and soft X-ray regions. A fourth spectroscopy beamline is installed on a bending magnet port where circularly polarized radiation can be used. A bending magnet beamline is also used for time resolved X-ray diffraction.

## MAX III Beamlines

Two undulator beamlines are operational at the 700 MeV MAX III storage ring; one EPU covers the low energy region 5 - 50 eV and a planar undulator covers the energy range 13 - 200 eV. The undulators serve beamlines for angular and spin resolved photoelectron spectroscopy. Operation of a third beamline for infra-red microspectroscopy, utilising bending magnet radiation, was started during 2013. ■

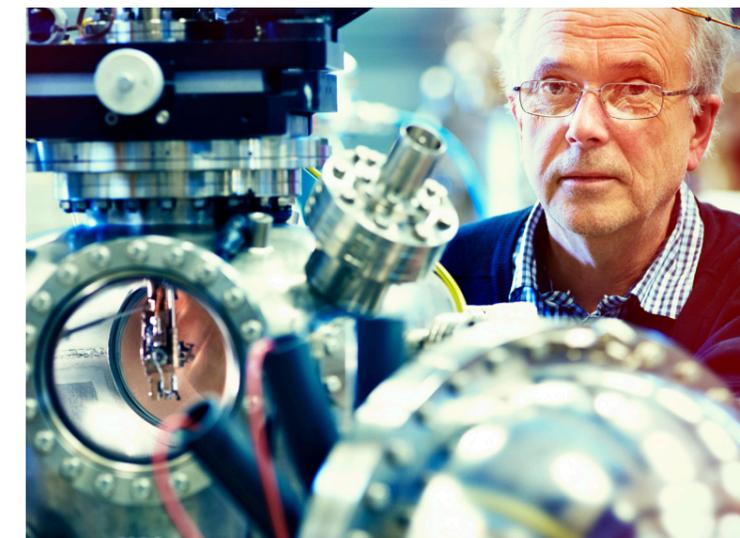


Table 1.

## MAX I Beamlines

Beam port	Source type	Beamline / Monochromator	Energy or wavelength range	Experimental techniques
NP	Tagged photon beam	Tagging spectrometer	15 - 185 MeV	Nuclear physics.

Table 2.

**MAX II Beamlines**

Beam port	Source type	Beamline / Monochromator	Energy or wavelength range	Experimental techniques
I311	Undulator	PGM (modified SX-700 with spherical focusing mirror)	43 - ~1500 eV	High resolution XPS, XAS, PEEM, LEEM
I411	Undulator	PGM (modified SX-700 with plane-elliptical focusing mirror)	40 - ~1500 eV	High resolution XPS, XAS, coincidence spectroscopy
SPECIES*	Elliptically polarizing undulator	Collimated PGM	27 - ~1500 eV	HPXPS branch: XPS, XAS, on solids under near ambient pressure conditions. RIXS branch: XAS, XES and RIXS
D611	Bending magnet	Be-windows, Double-crystal monochromator	2 - 10 keV	Time resolved XRD
I711	Multi-pole wiggler	Be-window, Bent Si(111) crystal	0.98 - 1.4 Å	Powder diffraction
I811	Superconducting multi-pole wiggler	Double-crystal monochromator. Exchangable Si(111) & Si(311) crystals	2.4 - 21 keV	EXAFS, XANES, Surface XRD and X-ray reflectivity
I911/1	Superconducting multi-pole wiggler	Diamond crystal, multi-layer mirror	Quasi-fixed wavelength, 1.2 Å	Presently used for education / test station
I911/2	Superconducting multi-pole wiggler	Bent Si crystal, multi-layer mirror	Fixed wavelength, 1.04 Å	Protein crystallography
I911/3	Superconducting multi-pole wiggler	Collimating mirror. Double-crystal monochromator. Focusing toroidal mirror	0.7 - 2.0 Å	Protein crystallography, with the MAD and SAD techniques
I911/4	Superconducting multi-pole wiggler	Bent Si crystal, multi-layer mirror	Fixed wavelength, 0.91 Å	SAXS
I911/5	Superconducting multi-pole wiggler	Diamond crystal, multi-layer mirror	Fixed wavelength, 0.9 Å	Presently used for education / test station
I1011	Undulator with variable polarization	Collimated PGM	200 - 2000 eV	MCD and related techniques for studies of magnetic materials
D1011	Bending magnet	PGM (modified SX-700 with plane-elliptical focusing mirror). Off-plane radiation for circular polarized radiation	40 - ~1600 eV	High resolution XPS, XAS, circular dichroism

\* Not yet operative

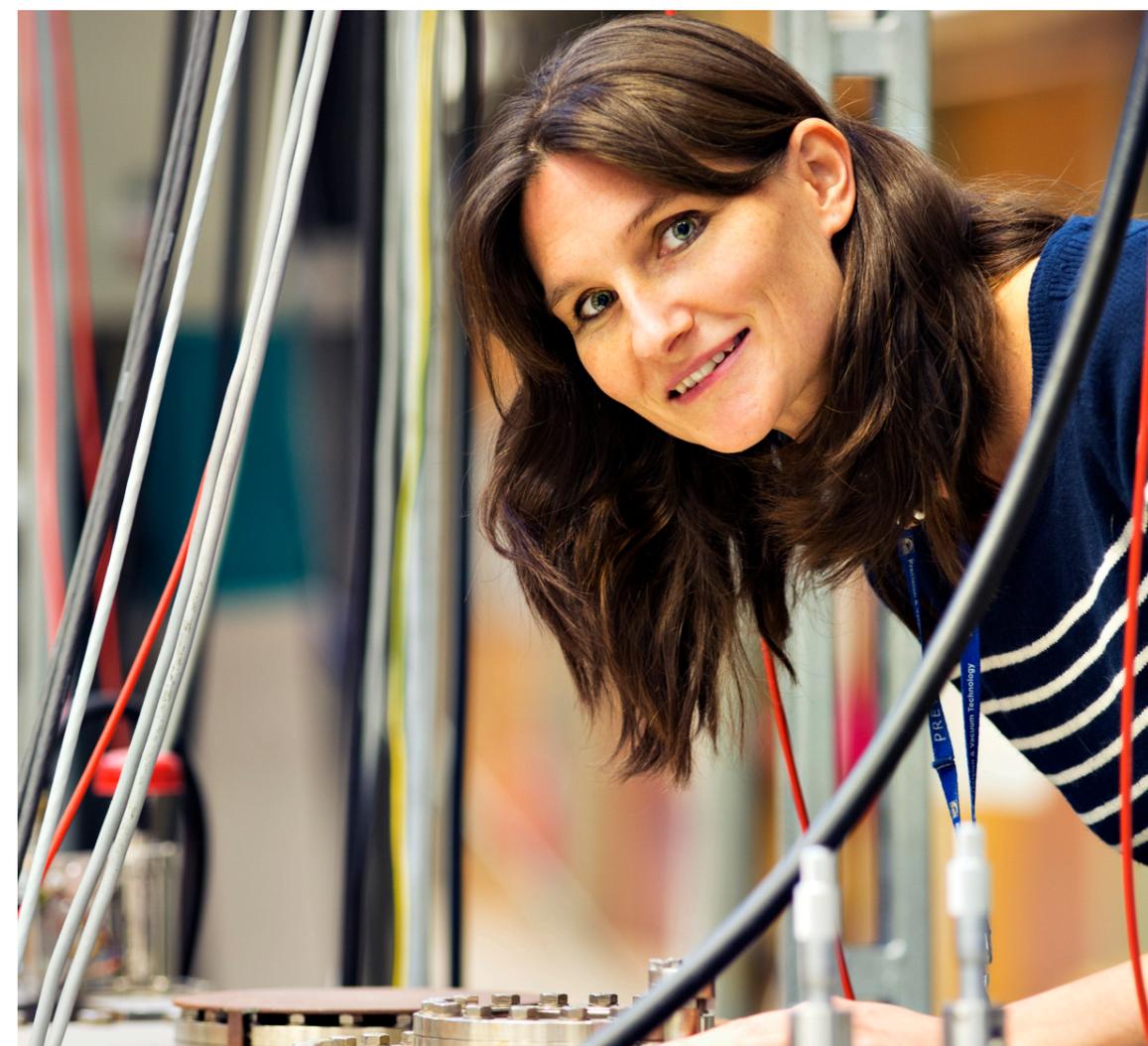


Table 3.

**MAX III Beamlines**

Beam port	Source type	Beamline / Monochromator	Energy or wavelength range	Experimental techniques
I3	Undulator with variable polarization	6.65 m Off-axis Eagle Type NIM	5 - 50 eV	High resolution (meV) angle- and spin-resolved PES on solids. On-line MBE system. Side branch for atomic and molecular spectroscopy, luminescence
I4	Undulator	5.5 - 5.8 m-SGM, 162°	13 - 200 eV	Angle-resolved photoemission
D7	Bending magnet	Transfer optics, FTIR spectrometer and IR microscope	12000 - 10 cm <sup>-1</sup>	Infrared microspectroscopy



# FASM – The Association for Synchrotron Radiation Users at MAX IV

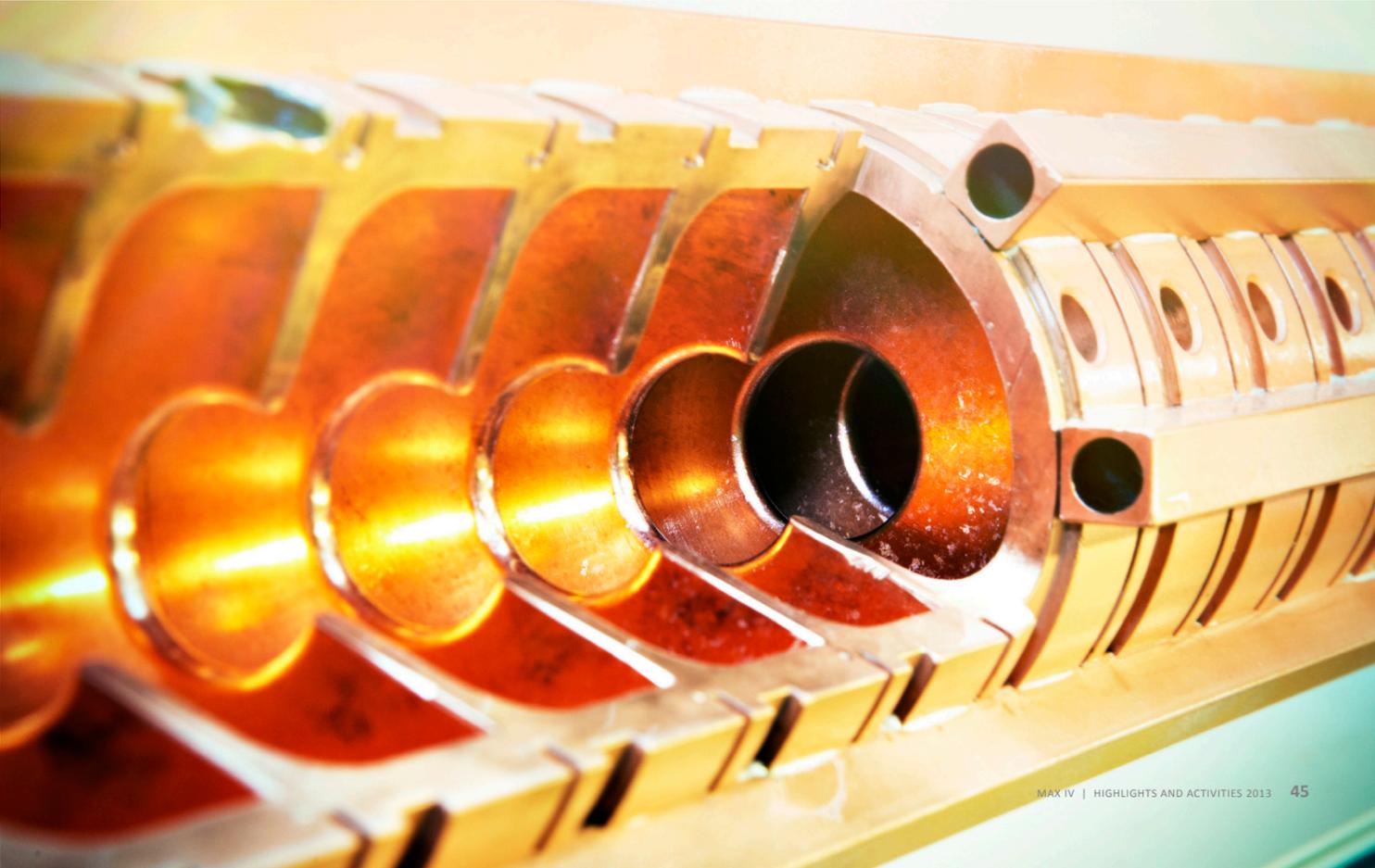
All users of the MAX-lab facility are by definition members of the FASM organisation. FASM aims at a broad participation involving all parts of the user community and at efficient communication with the MAX IV Laboratory board and management. Through FASM it is possible to communicate current and future needs within the user community and with the MAX IV Laboratory board and management. At the same time the association disseminates information to the users about the plans and prospects for MAX IV. FASM's mission is increasingly important as the user community is growing rapidly with more scientific disciplines actively using the present MAX-lab facility, and even more so for the upcoming MAX IV facility. In view of this, FASM will introduce a number of proposals aimed at strengthening the activities at MAX-lab, deepening the knowledge of the possibilities at the new MAX IV facility and furthering the aid to new users by the association.

The 26<sup>th</sup> annual meeting of The Association for Synchrotron Light Users at MAX IV ("Föreningen för Användare av Synkrotronljuset vid MAX-laboratoriet" or FASM) took place in connection with the Annual User Meeting on

November 23<sup>th</sup>, 2013 at Elite Hotel Ideon in Lund. A new FASM board for the upcoming three years was elected with Professor Raimund Feifel, Uppsala University, as chairman, and with Professors Marcus Agåker, Uppsala University, Keld Mortensen, University of Copenhagen, Britt-Marie Steenari, Chalmers University of Technology, and Susanna Törnroth-Horsefield, Lund University, as members. The previous FASM board with Professor Ingmar Persson, Swedish University of Agricultural Sciences, as chairman was warmly thanked for their efforts and achievements.

MAX-lab users, and anyone with interest in using the MAX IV facility, who want to bring up ideas to improve MAX-lab as scientific tool and MAX IV as organisation are welcome to contact:

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# FACTS AND FIGURES

## The Organisation

The MAX IV Laboratory was created 2010 through an agreement between Lund University, the Swedish Research Council, VINNOVA and Region Skåne. The MAX IV Laboratory is a national facility according to SFS 1994:946 (revised 2011:1567). The creation of the MAX IV Laboratory has recently been accompanied by changes in order to handle the rapidly growing organisation.

The overall responsibility for the laboratory resides with the Board chaired by Professor Lars Börjesson until late fall 2013 and thereafter by Professor Hans Hertz. The most recent term of office for the Board ended during 2013 and some new members were chosen for the new term. Members of the present Board is listed in table 1.

Lund University, and its board, is hosting the MAX IV Laboratory. The major funders of the operations; the Swedish Research Council and Lund University, regulates its commitments in multi-year agreements.

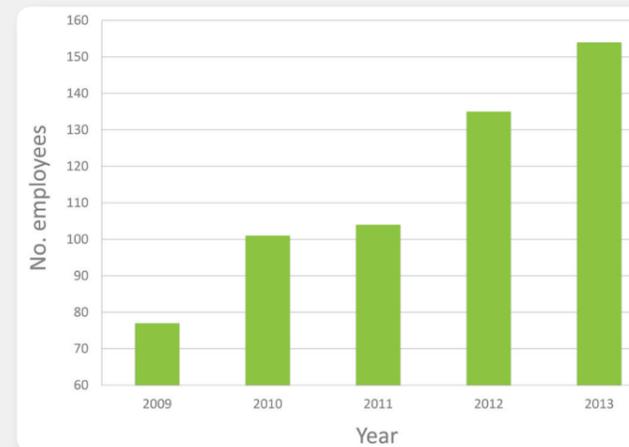
The operation of the MAX IV Laboratory is led by the management team comprised of the Director, the Physical Science Director, the Life Science Director, the Machine

Director and the Administrative Director. During 2013 the line organisation has been developed with formal groups led by group managers. This will for example unload the management team in staff matters and facilitate a more effective internal communication.

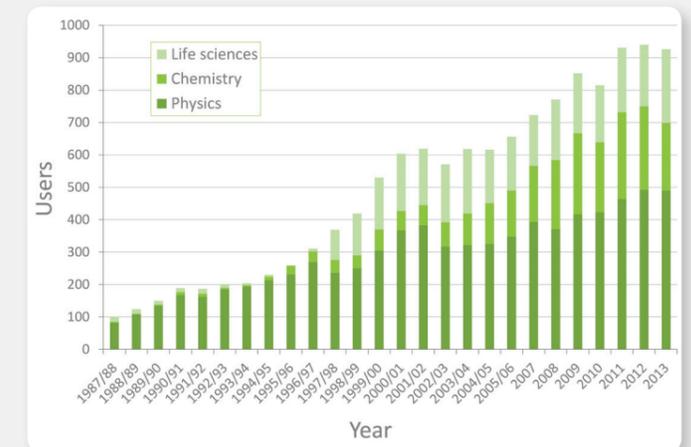
The budget of the MAX IV Laboratory is divided into two separate parts, one for the operation of the existing MAX-lab facility and the other for the construction of MAX IV. The operation budget was 122 MSEK in 2013. The majority of the funding was provided by the Swedish Research Council, while the host institution Lund University covered the rent, electricity and water costs.

The growth in the number of employees shown in Figure 1 is due to both the MAX IV project and a strengthening of the support to users at MAX-lab. The majority of the staff is engaged both in the operation of MAX-lab and in the MAX IV related projects.

The staff is becoming more and more international and in the end of 2013 more than 20 nationalities were represented among the laboratory personnel.



**Figure 1.** Number of employees at the MAX IV Laboratory. Presented figures are end of the year data.



**Figure 2.** Number of MAX I, II and III users per year and discipline. The 1987/88 to 2004/05 numbers are July to June figures. The 2005/2006 value indicates number of users from June 2005 to end of 2006.

### MAX-lab Users

The number of proposals submitted for beamtime continues to increase and in 2013 more than 350 applications were received (Figure 3). Proposals are reviewed by the Program Advisory Committees (PAC), who also recommends the amount of allocated beamtime. Research performed at MAX-lab results in the publication of around 200 research papers every year.

During 2013 more than 900 scientists performed experiments at MAX-lab. The scientific projects included experiments in atomic and molecular physics, solid state physics, surface physics, material science, chemistry, life science and environmental science. The majority of the experiments have been performed on the MAX II and MAX III storage rings. The researchers represented 160 different industrial, academic and government laboratories from 35 different countries (Figure 4). The number of visiting researchers follows the strong trend, observed over more than twenty years, of a diverse and expanding user community (Figure 2).

Table 1.

### Board

Hans Hertz (chair), Royal Institute of Technology, Sweden \*  
 Helmut Dosch, DESY, Germany  
 Kristina Edström, Uppsala University, Sweden  
 Anne l'Huillier, Lund University, Sweden  
 Helena Malmqvist, Corporate Research, ABB  
 Richard Neutze, Göteborg University, Sweden  
 Ulf Olsson, Lund University, Sweden  
 Michel van der Rest, former CEO SOLEIL, France  
 Marianne Sommarin, Umeå University, Sweden

\* Succeeding Lars Börjesson, Chalmers University of Technology, Sweden from December 2013

Table 2.

### Management Group

Christoph Quitmann, Director  
 Mikael Eriksson, Machine Director  
 Jesper Andersen, Physical Science Director  
 Peter Andersson, Administrative Director  
 Tomas Lundqvist, Life Science Director

Table 3.

### Scientific Advisory Committee (SAC)

Joseph Nordgren (chair), Uppsala University, Sweden  
 Rafael Abela, PSI, Swiss Light Source, Switzerland  
 Alfons Molenbroek, Haldor Topsoe A/S, Denmark  
 Harald Reichert, ESRF, France  
 Gebhard Schertler, PSI, Swiss Light Source, Switzerland  
 Phil Woodruff, University of Warwick, UK  
 Kristina Djinojic-Carugo, Max F. Perutz Laboratories, Austria  
 Keijo Hämäläinen, University of Helsinki, Finland  
 Lise Arleth, University of Copenhagen, Denmark  
 Alexander Korsunsky, University of Oxford, UK  
 Philip Hofmann, Aarhus University, Denmark  
 Ivan Vartaniants, University of Hamburg, Germany

Table 4.

### Machine Advisory Committee (MAC)

Lenny Rivkin (chair), PSI, Swiss Light Source, Switzerland  
 Klaus Balewski, DESY, Germany  
 Peter Kuske, Helmholtz Zentrum Berlin, Germany  
 Søren Pape Møller, Aarhus University, Denmark  
 Richard Walker, Diamond, UK  
 Bob Hettel, SLAC, USA

The Machine Advisory Committee (MAC) and Science Advisory Committee (SAC) both provide valuable advice to the Management and Board of the MAX IV Laboratory.

Table 5.

### Program Advisory Committee (PAC)

Lars Johansson (chairperson), Karlstad University, Sweden

#### Soft X-ray and IR science

Anne Borg, Norwegian University of Science and Technology, Norway  
 Wendy Flavell, The University of Manchester, UK  
 Carol Hirschmugl, University of Wisconsin–Milwaukee, USA  
 Karsten Horn, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany  
 Maya Kiskinova, ELETTRA, Italy  
 Marko Huttula, University of Oulu, Finland  
 Catalin Miron, SOLEIL, France  
 Luc Patthey, PSI, Swiss Light Source, Switzerland  
 Cinthia Piamonteze, PSI, Swiss Light Source, Switzerland  
 Wilfried Wurth, University of Hamburg, Germany

#### X-ray science

Jean Daillant, SOLEIL, France  
 Kristina Djinojic-Carugo, The Max F. Perutz Laboratories, Austria  
 Andrew N. Fitch, ESRF, France  
 Henning Friis Poulsen, Risø-DTU, Denmark  
 Mikael Gajhede, University of Copenhagen, Denmark  
 Ragnvald Mathiesen, Norwegian University of Science and Technology, Norway  
 Moniek Tromp, Technical University of Munich, Germany

Figure 3. Number of submitted and approved proposals for beamtime at MAX I, II and III per year.

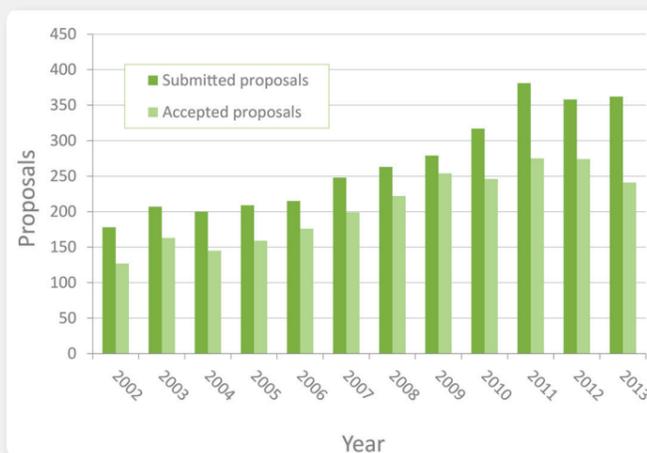


Figure 4. Allocated beamtime versus origin of the applicant for the year 2013.

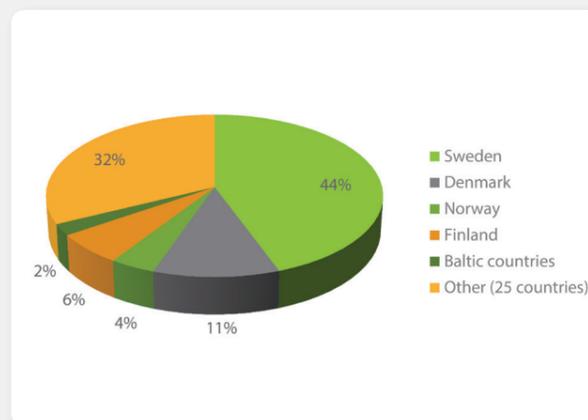


Figure 5. Number of publications with data from measurements at the MAX IV Laboratory per year and discipline.

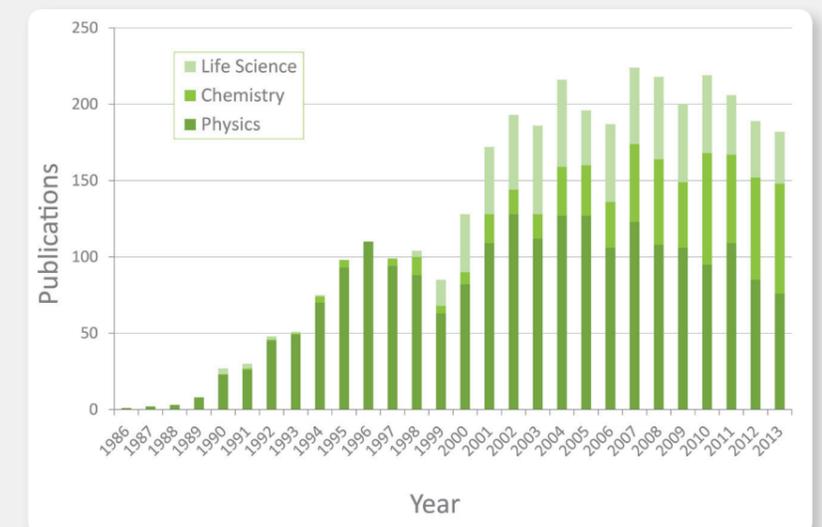


Table 6.

**MAX IV Laboratory Industrial Network Group (MING)**

Ulf Karlsson, Royal Institute of Technology, Sweden  
 Jan Lif, Stora Enso Renewable Packaging, Sweden  
 Per Wiklund, Nynäs AB, Sweden  
 Jonas Gurell, Swerea AB, Sweden  
 Susanne Norgren, Sandvik Mining, Sweden  
 Hanne Benedicte Rasmussen, Novo Nordisk A/S, Denmark  
 Tove Sjögren, AstraZeneca, Sweden  
 Anna Stenstam, Colloidal Resource AB, Sweden  
 Mats Qvarford, Tetra Pak Packaging Solutions AB, Sweden

Table 7.

**University Reference Group (URG)**

Alf-Erik Almstedt, Chalmers University of Technology, Sweden  
 Aleksandar Matic, Chalmers University of Technology, Sweden  
 Jens Birch, Linköpings University, Sweden  
 Per Danneun, Linköpings University, Sweden  
 Anders Karlhede, Stockholm University, Sweden  
 Lennart Bergström, Stockholm University, Sweden  
 Luca Jovine, Karolinska Institutet, Sweden  
 Gunter Schneider, Karolinska Institutet, Sweden  
 Björn Birgisson, Royal Institute of Technology, Sweden  
 Ulf Karlsson, Royal Institute of Technology, Sweden  
 Olof Karis, Uppsala University, Sweden  
 Gunnar Ingelman, Uppsala University, Sweden  
 Richard Neutze, Göteborg University, Sweden  
 Stefan Hohmann, Göteborg University, Sweden  
 Marianne Sommarin, Umeå University, Sweden  
 Per Persson, Umeå University, Sweden  
 Lars Johansson, Karlstad University, Sweden  
 Alexander Soldatov, Luleå University of Technology, Sweden  
 Erik Höglund, Luleå University of Technology, Sweden  
 Crister Ceberg, Lund University, Sweden  
 Klas Malmqvist, Lund University, Sweden  
 Torbjörn von Schantz, Swedish University of Agricultural Sciences, Sweden

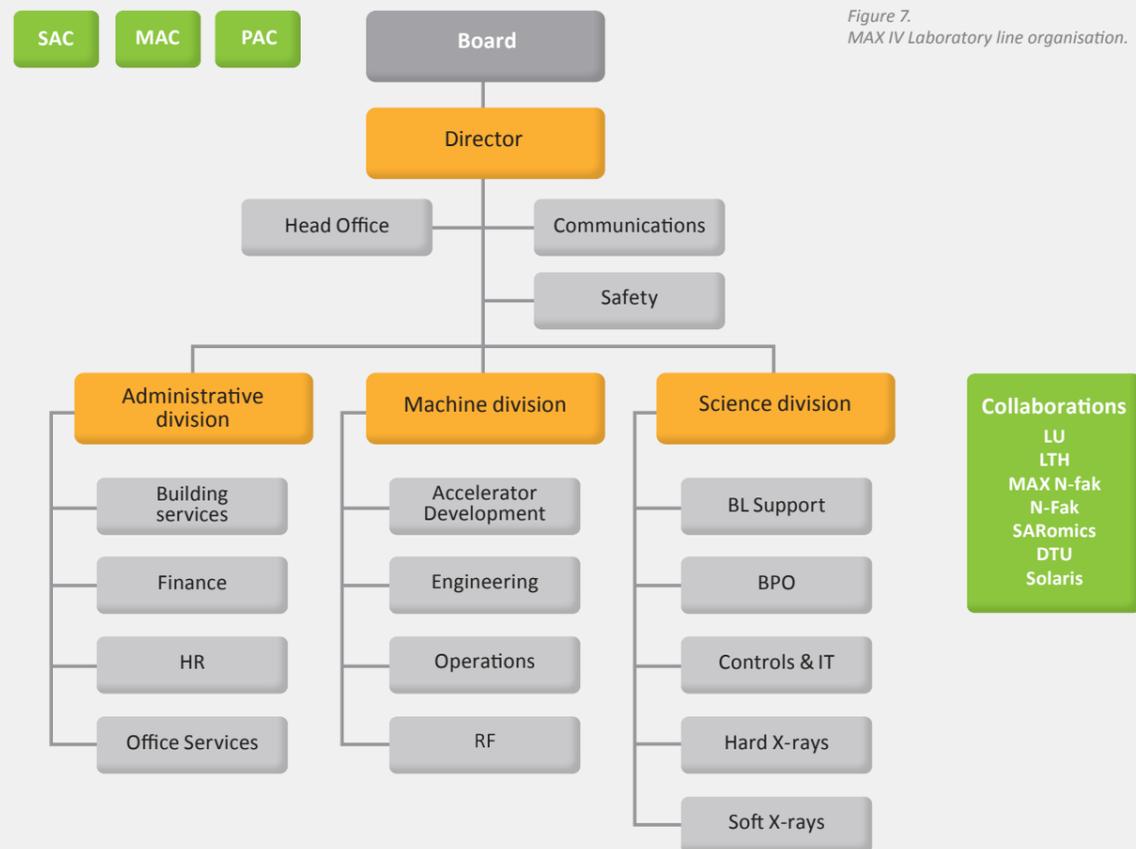


Figure 7. MAX IV Laboratory line organisation.



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