# SPECIES

**MAX IV beamline review report**

Esko Kokkonen, Alexander Klyushin, Conny Såthe, Calley Eads, Rosemary Jones, Margit Andersson, Anirudha Ghosh, Takashi Tokushima, Mihai Pop, Louisa Pickworth, Andrey Shavorskiy

2024-04-27

# Table of contents

# 1 General introduction

SPECIES is a soft X-ray beamline on the 1.5 GeV ring at the MAX IV Laboratory. It covers a wide photon energy range of 30 – 1500 eV with variable polarization. There are two branches, each with their own permanently installed endstation. Branch A has an endstation dedicated to ambient pressure X-ray photoelectron spectroscopy (APXPS) and branch B to resonant inelastic X-ray scattering (RIXS). In addition, both branches can carry out X-ray absorption spectroscopy (XAS) measurements using signals from various sources. The optics are similar on both branches providing a moderately focused beam for APXPS (~100 µm) and a tighter focus for RIXS (~10 µm). The beamline covers an energy resolution typical for soft X-ray beamlines of resolving power values on the order of 5000 – 10000 over nearly the entire photon energy range.

SPECIES has been designed to cover a large range of scientific topics between both endstations. The APXPS endstation is available to any users interested in investigating the structure-function relationships of surface-gas reactions, *i.e.* how surface structure on the atomic scale influences the material reactivity towards gases. The need to conduct such measurements on complex, functional materials with realistic *in situ* and *operando* conditions is an important line of development in today's material research and shows ever increasing popularity among many fields. RIXS, on the other hand, is able to give a complementary view into material properties by increasing the fundamental understanding of vacuum ultraviolet and soft X-ray scattering. While the elementary knowledge of light-matter interactions is important on its own right, the beamline also establishes the necessary foundation for the employment of RIXS to many kinds of applied research concerning functional materials, complex functional molecules, etc.

The beamline was designed to be a general-purpose platform for many different user communities. This aspect mainly originates from the flexibility of the sample environments which are, on both endstations, designed to cater to a large array of experiments. The APXPS endstation has sample environments allowing experiments in the fields of catalysis research, material characterization, thin film deposition, etc. utilizing dedicated cells. The endstation is equipped with many common surface preparation tools enabling the investigations using model systems and surface science. The studies can be carried out both in (near-)ambient conditions but also under UHV conditions. The endstation is equipped with complementary instruments (*e.g.* mass spectrometers) mainly allowing to probe gas phase products and connect this information easily to the XPS data acquired from the surface. On the RIXS endstation, several different exchangeable sample environments (called "sample rods") exist that are designed for different types of experiments. The capabilities of these sample environments allow for heating or cooling samples, creating gaseous environments, applying bias voltages, or focusing solely on gas phase RIXS. However, in practice, nearly all the RIXS experiments have been dedicated to investigating solid materials in UHV.

Most of the above-mentioned capabilities are currently considered to be baseline operations of the beamline and are offered to all users through the general MAX IV proposal calls. In addition, there are several ongoing development projects to improve the beamline and endstation capabilities by extending the sample environments but also improving the production of X-rays to exploit the full potential of the beamline. Development projects are commonly realized through collaborations with experts from universities or other institutes and the researchers involved will often have a chance to participate in in-house research activities as well.

In the MAX IV Science Division organization, SPECIES beamline falls under the Spectroscopy II group. In addition, the staff working at SPECIES beamline belong to the APXPS and RIXS teams, operating the branches of the SPECIES beamline as well as the HIPPIE and Veritas beamlines for APXPS and RIXS, respectively. The SPECIES beamline is co-managed by the two teams, with some staff being full time-dedicated to the beamline while others working only part-time at SPECIES. The beamline flourishes from the strong connection to the HIPPIE and Veritas beamlines. Not only does this collaboration extend the knowledge sharing within the teams, but also lead to the availability of complementary beamline equipment and sample environment capabilities. While SPECIES excels at lower photon energies, both HIPPIE and Veritas extend the available photon energy range for APXPS and RIXS towards 2000 eV and beyond. For APXPS, the sample environments are quite different at SPECIES and HIPPIE, for instance, HIPPIE has an entire branchline dedicated to the

investigation of liquid-solid interfaces, thus enabling deeper specialization for specific experiments. For RIXS, however, the "sample rods" are fully exchangeable with Veritas RIXS endstation, enabling near-seamless experiments on both beamlines.

We believe the beamline is mature in most aspects, has well-established user communities, and is attractive to new users. The oversubscription level is often at about 2, which at present seems to be healthy level for the beamline. In addition to the on-going developments to improve the beamline (as mentioned above and detailed later in this document), our ambition is to increase the overall user satisfaction level at the beamline. Bearing this in mind, the development projects should be strategic in order to maintain an active user community that is able to use the beamline to further their respective research directions in the most optimum manner.

# 2 Technical description

## 2.1 Beamline design

The X-rays are generated using an elliptically polarizing undulator EPU61 of APPLE-II type[1] with 41.5 periods and a period length of 61 mm. During commissioning and operation, it has been demonstrated that the undulator can operate without disturbing the stored electron beam down to the lowest gap of 14 mm, which corresponds to a $K_{max}$ of 5.56 and yields the lowest photon energy range of 30 eV. The highest available photon energy is approximately 1500 eV. For polarizations other than horizontal, the available photon energy range is slightly narrower. The brilliance produced by the EPU61 is presented in Figure 1~~Figure 1~~. Currently, only horizontal and vertical polarizations are used in day-to-day experiments. While circular and inclined polarizations are technically available, they have not been fully characterized due to very low demand from users.

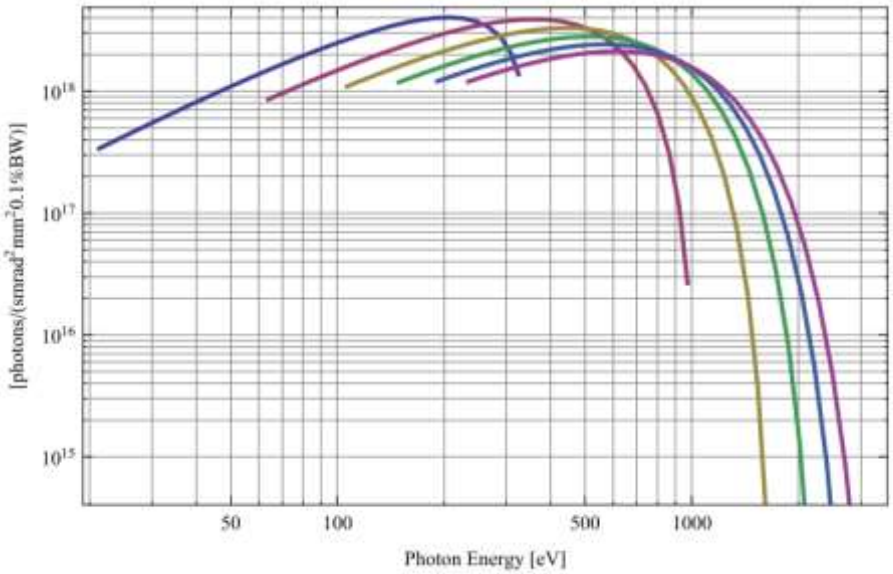


Figure 1: Calculated brilliance in the 1st, 3rd, 5th, 7th, 9th, and 11th harmonics at the peak energy of the synchrotron radiation emitted by EPU61 in the planar mode.

The beam enters the optical hutch through the front end where some of the beam is skimmed in order to only illuminate the active area on the first mirror (M1, cylindrical). Note that the front ends of all the beamlines in the 1.5 GeV ring are standardized with nearly identical components. The front end comprises

[1] E.J. Wallén *et al.*, Proceedings of the 5th Int. Particle Accelerator Conf. **IPAC2014**, 3 pages (2014)

the fixed aperture photon mask and the so-called movable masks which can be used to select certain portions of the beam to enter the rest of the beamline. The most important components in the front end are a water-cooled heat absorber that can take the full heat load of the beam, a bremsstrahlung photon beam shutter and a fast-closing valve.

The M1 mirror collimates the radiation vertically. Additional baffles after the M1 (beam defining aperture, BDA) define the beam for correct illumination for the monochromator optics. The beam is then monochromatized using a plane-grating monochromator (cPGM). Only one grating with 1221 lines/mm is currently in use which covers the entire photon energy range. Figure 2~~Figure 2~~ shows the layout of the beamline together with distances from the source. The monochromator optics consist of the plane mirror (M2) and the plane grating (PG).

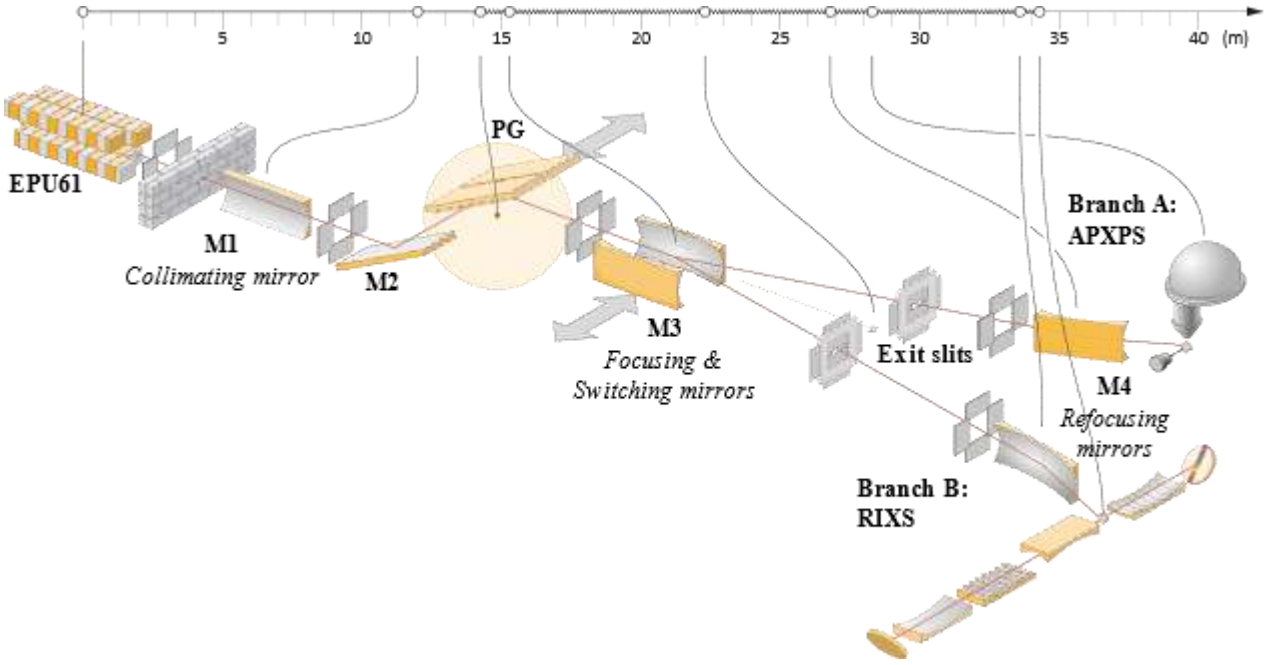


Figure 2: SPECIES beamline layout showing the major optical components and their distance from the source.

Downstream of the monochromator, two focusing mirrors (M3, toroidal) are placed facing each other. Either one can be moved into the beam in order to choose which branch should receive the light. Each branch has its own continuously adjustable exit slit and refocusing optics (M4, ellipsoidal for RIXS, toroidal for APXPS), which are very different. For RIXS, a small spot (a few tens µm) with high photon density is required whereas for APXPS a larger spot (~100 µm) with uniform illumination and a spot size independent of the slit is preferred. For the APXPS branch, the requirement of constant spot size is achieved using a toroidal M4 mirror, which focuses the beam horizontally to the sample location, but places the vertical focus tens of mm beyond the sample. Using this so-called astigmatic focusing, the vertical beam size is more dependent on the divergence of the source rather than its size and makes it possible to achieve a near constant beam size, independent of the exit slit opening. The RIXS branch has an ellipsoidal refocusing mirror, which yields a good spot size, so that the energy resolution required by the endstation spectrometers is not compromised.

The beamline design has been further detailed in two papers, which contain much more detail on the optical elements, their design choices, and many more.[2,3]

[2] S. Urpelainen *et al.*, J Synchrotron Rad **24**, 344 (2017).
[3] E. Kokkonen *et al.*, J Synchrotron Rad **28**, 588 (2021).

## 2.2 Beamline performance

### 2.2.1 Flux

The beamline flux has been measured on the photodiode located on the beam diagnostic unit between the exit slit and M4 mirror in the APXPS branch. The flux curve measured using horizontal polarization and at a fixed slit opening of 50 µm is seen in Figure 3~~Figure 3~~. The measurement was done using the typical settings (*e.g.* BDA opening of 4x2 $mm^2$) that are routinely used during user operation. An exit slit of 50 µm represents the normal exit slit opening used by nearly all APXPS users. It gives an approximate resolving power of 6000 at 400 eV, a value that is often deemed acceptable in most experiments.

The beamline flux is also calculated and simulated using a combination of Spectra and RAYUI. For the calculations, a realistic roughness value of 1.2 nm for the optics was chosen. The calculated beamline flux is closer to design values at lower energies, but it overestimates the delivered flux at higher energies. This deviation could be accounted for by a number of factors not included in the simulation:

- Carbon contamination on the optical components. This contamination is mitigated using $O_2$ cleaning on the monochromator by continuously leaking $O_2$ into the vacuum chamber, however a significant carbon dip still persists. This might originate from the other optics besides the M2 and the grating but could also be due to the insufficient removal of carbon from M2 and the grating.
- Increased roughness on the optics due to 1) constant $O_2$ dosing and 2) ozone cleaning. The optics are also quite old, further increasing the likelihood of having higher roughness. Roughness on optical surfaces results in lower flux for all photon energies but the effect is pronounced at higher energies.
- M1 has visible damage on the Au coating.
- Imperfect alignment.
- Aged and potentially carbon coated photodiode.

Some of the above-mentioned points can be easily solved (*e.g.* new photodiode), while for others (new optical components) different solutions exist. These are specified later in development projects.

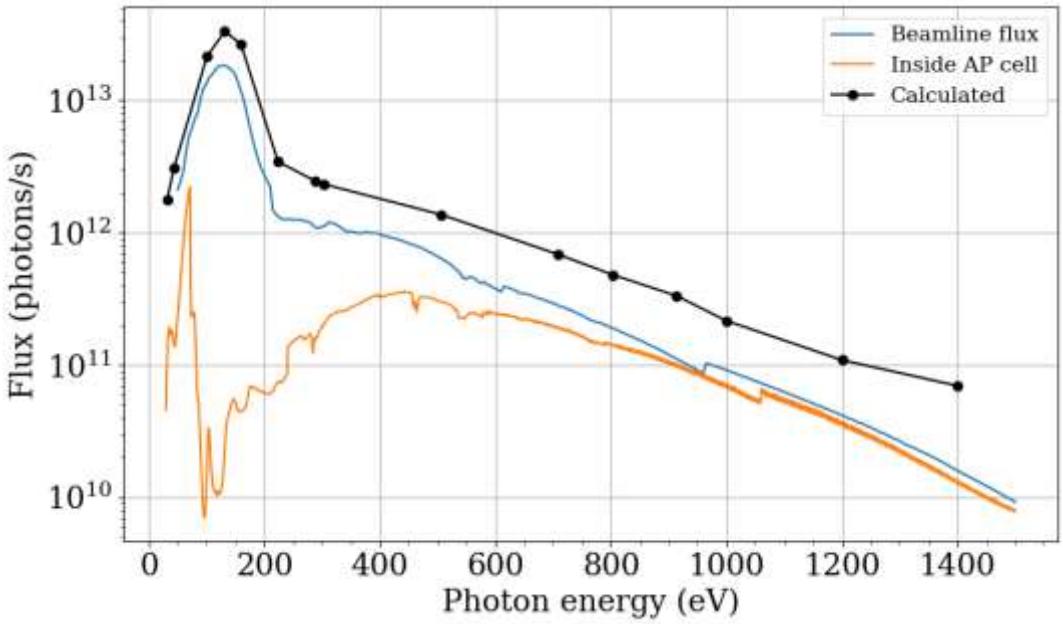


Figure 3: Flux curve measured with a constant slit of 50 µm with horizontal polarization and using the common beamline settings used in typical user operation. The beamline flux is measured before the final refocusing mirror and inside the ambient pressure (AP) cell in the APXPS endstation. In the latter case the Al window reduces the flux at certain energies. The calculated flux is also shown.

### 2.2.2 Resolution

A typical beamline resolution is shown in Figure 4~~Figure 4~~ measured with nitrogen and neon gases at ~45 eV (Ne I resonance), ~401 eV (N K-edge), and ~867 eV (Ne K-edge). With these two gases it is possible to measure the resolution over a large energy range, while the N K-edge absorption is also used to make the absolute energy calibration of the monochromator. The measurements have been done using a typical beamline exit slit setting of 50 µm. As can be seen in Figure 4~~Figure 4~~, decent photon energy resolutions are achieved across a wide range of photon energies while maintaining high flux values. At lower photon energies the flux increases significantly, typically requiring a reduction in the slit size to prevent saturation of the detectors. At lower photon energies the beamline resolution is not usually important since the total resolution is often dominated by the detecting instruments (approximately hundreds of meV for XPS using typical settings).

Resolution measurements shown in Figure 4~~Figure 4~~ were measured in the small volume beamline gas cell located just after the exit slit. The gas cell volume is isolated between two Al membranes with a thickness of about 200 nm. This allows gas pressurization of this section of the beamline up to $10^{-2}$ mbar. The gas cell is equipped with instrumentation to enable measurement of gas phase total ion yields. All resolution measurements were taken with a monochromator $C_{ff}$ value of 2.25 and they match very well the values expected from simulations/calculations for the monochromator.

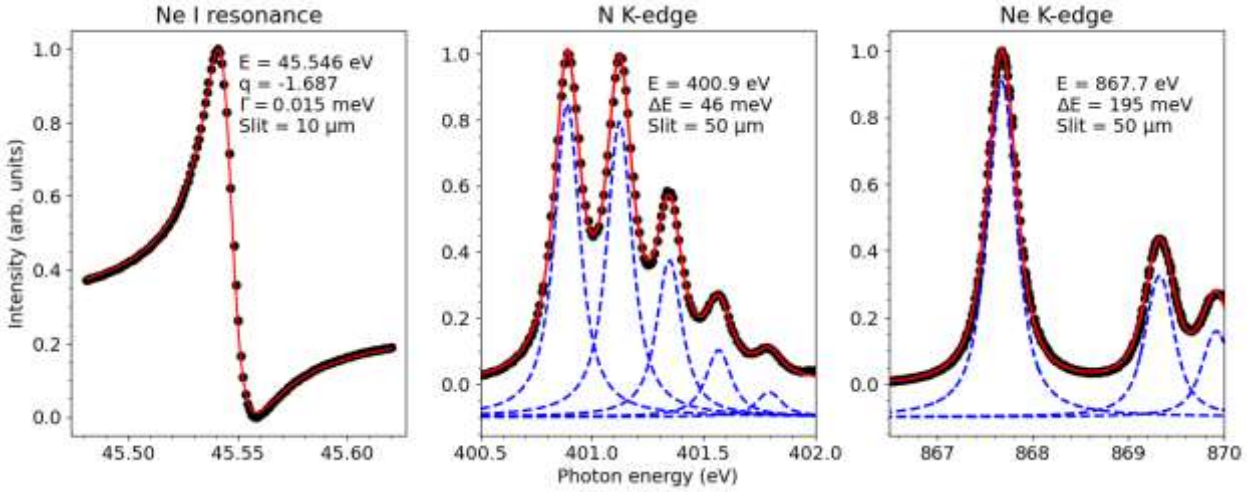


Figure 4: The measured beamline energy resolution at Ne I resonance, N K-edge, and Ne K-edge. The Ne I resonance measurement was done at a small slit of 10 µm in order to showcase the typical achievable resolution, while the N and Ne K-edges are at 50 µm which is more typical for those energies. The N and Ne K-edge fits used fixed Lorentzian widths of 120 meV and 254 meV, respectively.

### 2.2.3 Spot size

The X-ray spot size inside the APXPS endstation is achieved a single final focusing mirror, $M4_{APXPS}$. An astigmatic focus was chosen to allow some insensitivity in the focal spot vertical distribution to the opening size of the exit slit. The beam focuses tangentially to the sample plane, but sagittally, $M4_{APXPS}$ focuses behind the sample by approx. 60 mm. This allows the exit slit to control the energy resolution and photon density on the sample without changing the sample illumination size[4]. The measured spot size in the APXPS endstation is highlighted in Figure 5~~Figure 5~~, which shows the projected spot size. The spot size was measured at three different energies, which shows that it does change slightly depending on the energy. A typical size is therefore roughly 120 µm horizontally and 60 µm vertically. This measurement was carried out with the sample normal towards the electron analyzer, i.e. 54.7° with respect to the beam, in other words it is the projected size of the beam. A larger spot size would require moving the APXPS endstation along the beam,

[4] W. Grizolli, *et al.*, J. Phys.: Conf. Ser. **425**, 152005 (2013).

which is practically infeasible. However, we see that due to diffraction, the beam size increases dramatically as the slit size approaches 0 mm (see Figure 5~~Figure 5~~).

The RIXS endstation has much stricter requirements for the spot size while also requiring minimal reflection losses. But, similarly to the APXPS branch, only a single elliptically refocusing mirror solution was adopted in order to achieve high incident beam flux. The $M4_{RIXS}$ mirror is placed 700 mm away from the sample to allow high demagnification of about 16. The spot size is approximately 25 µm horizontally and about 5 µm vertically. The exit slit size defines the vertical spot size. Aligning the sample to the best focus of the beamline is an important task when setting up a new RIXS experiment. To do this, the high-accuracy, high-stability sample manipulator is used together with a simple focus finder developed by the RIXS team. This also means the spot size can be easily verified as part of the weekly set-up of the beamline.

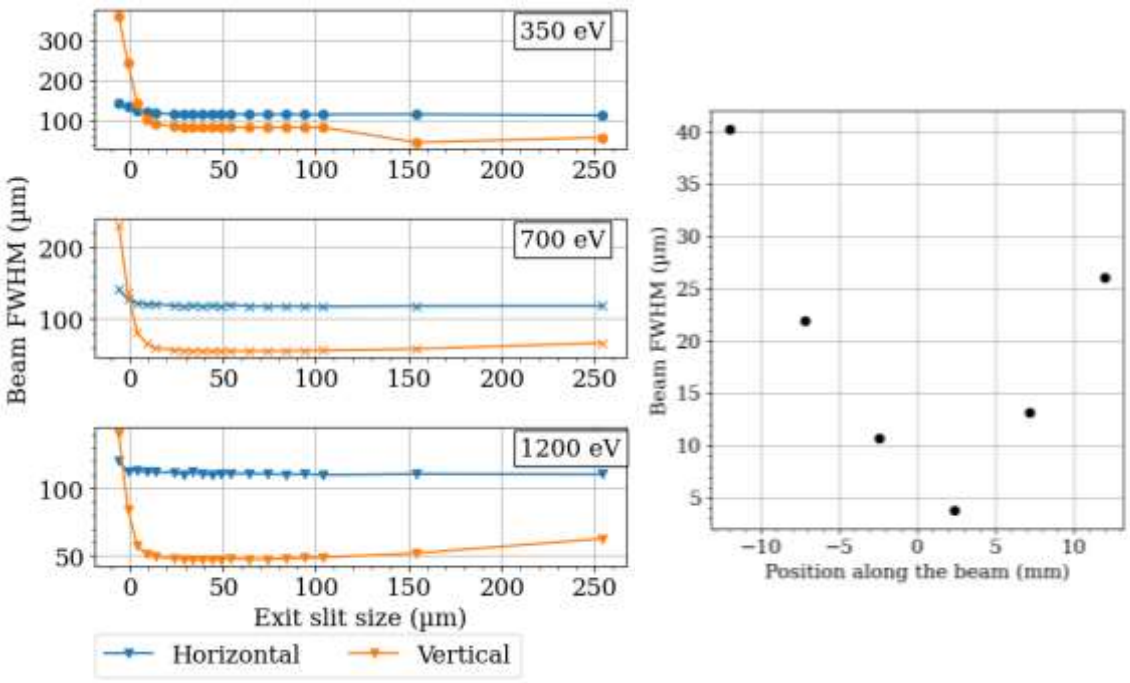


Figure 5: Left: The FWHM value of the projected spot size horizontally and vertically as measured in the APXPS endstation at three different energies. Right: The FWHM values of the vertical spot size measurements along the beam path. The data is measured at photon energy of 399 eV.

## 2.3 Endstation A (APXPS endstation)

The APXPS endstation is dedicated to *in situ* and *operando* studies of solid-gas interfaces at ambient pressure conditions using XPS, Auger electron spectroscopy (AES) or XAS in the soft X-ray region. The endstation features a special dockable and retractable ambient pressure (AP) cell which is housed inside the analysis chamber (this is known as the Lund cell design or "cell-in-cell" concept). This feature therefore enables the user to carry out conventional ultrahigh vacuum (UHV) studies in addition to ambient pressure experiments. Switching between UHV and ambient pressure experiments can be done in a matter of minutes (depending on pump-out time of the used gas) without breaking vacuum, making it possible to prepare and characterize the surface before performing ambient pressure experiments. Briefly, the setup consists of three main chambers: load lock, preparation, and analysis chambers with an exchangeable AP cell and the ambient pressure electron energy analyzer (Figure 6~~Figure 6~~).

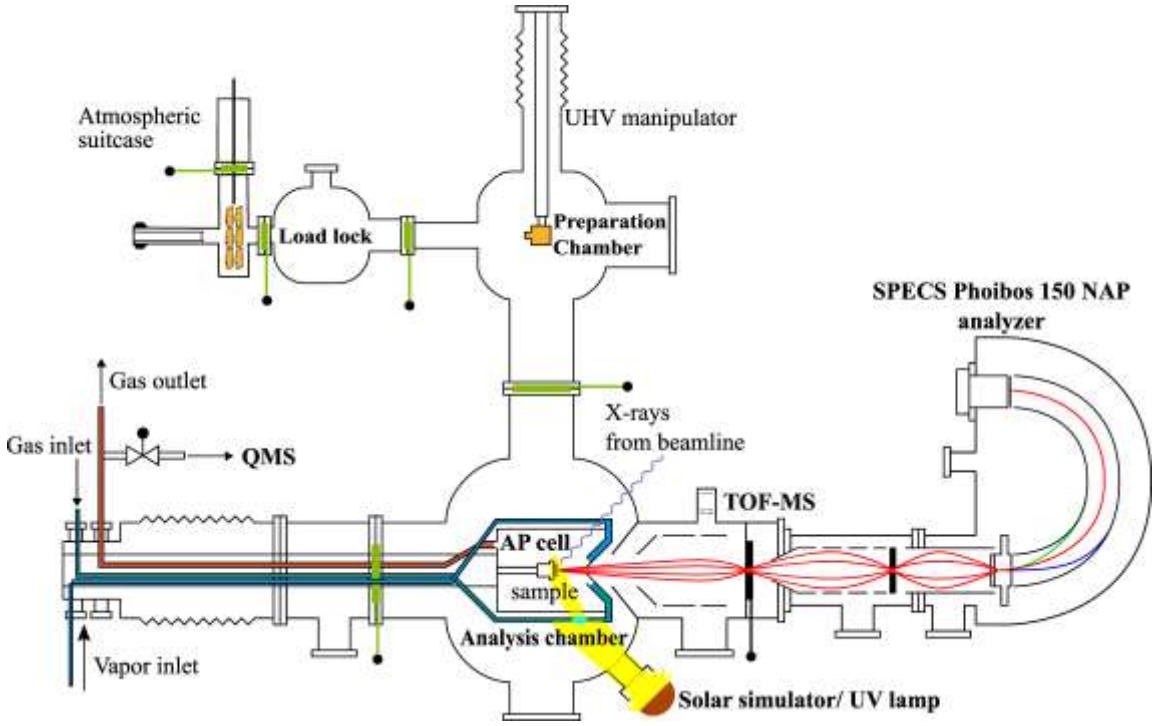


Figure 6. Schematic layout of the APXPS endstation. The endstation consists of a load lock chamber with a quick access door for introducing samples into the chamber, a preparation chamber with an UHV manipulator and option to attach user equipment, and the analysis chamber which houses the AP cell.

The AP cell itself can be changed with relative ease (in about 4 hours by two people), allowing studies using various sample environments that might require different configurations from the AP cell, such as different sample materials, sizes, geometries, etc. User modified or supplied AP cells are also possible to mount on the system. This makes the setup very versatile and facilitates studies within several disciplines such as catalysis, corrosion, thin film growth, and others.

### 2.3.1 Load lock and preparation chambers

The load lock chamber has a quick access door and a horizontal transfer to the preparation chamber which facilitates the quick loading of samples into the endstation vacuum system. Samples can be loaded one at a time. Additional sample loading equipment can also be attached to the load lock chamber. These include either UHV suitcases (for transferring samples under vacuum) or “atmospheric” suitcases. The atmospheric suitcase has 6 slots for SPECS/Omicron-style sample plates and allows sample transfer to the experimental station without exposure to air. In fact, air-sensitive samples can be transferred directly from a glove box or another setup to the load lock or vice versa.

The preparation chamber is equipped with an $Ar^+$ ion gun for sputtering, low-energy electron diffraction (LEED) system for surface structure characterization and an open port for user equipment. In order to carry out the required treatment, the preparation chamber also features three separate gas lines connected by a common leak-valve. The preparation chamber houses the UHV manipulator placed on the top of the chamber, which has an electron bombardment type sample heater allowing sample heating up to 1000 °C. The vertical connection to the analysis chamber makes it possible to use only one manipulator for both sample preparation and UHV measurements, making the sample transfer simple.

### 2.3.2 Analysis chamber

The analysis chamber is located right underneath the preparation chamber and is connected to the beamline. Measurements can be carried out either directly in the UHV manipulator, or in the ambient pressure (AP) cell. The analysis chamber additionally has some storage space for samples, allowing quickly changing the

measured sample. The beamline section connected to the analysis chamber contains a differentially pumped section and a line-of-sight ion pump, which together allow backfilling the chamber to pressures of up to ~$10^{-5}$ mbar without compromising the vacuum of the beamline.

The analysis chamber can also be equipped with a non-monochromatic twin magnesium and aluminum X-ray anode. The X-ray anode is primarily used for off-line measurements during times when synchrotron radiation is not available. However, the X-ray anode is often not installed, and therefore its use requires careful planning as the installation takes approximately one day.

Instead of the X-ray anode, the same port is often used for external (visible) light sources. The beamline has two light sources available for all users: a HAL-320W solar simulator from Asahi Spectra with a custom light guide and a Xe lamp model L6605 from Hamamatsu. Either light source can be attached to a CF40 viewport which has UV grade fused silica window. Each light source can be used with either the UHV manipulator or the AP cell. Figure 7~~Figure 7~~ schematically shows the alignment between the external light sources, the beamline and the analyzer nozzle. The angle between the external light source and the sample surface is 69˚. At the same time, the electron analyzer is placed at a "magic" angle of 54.7° with respect to the horizontally polarized X-rays.

Operation of either the solar simulator or the Xe lamp requires good transmission into the vacuum chamber and subsequently the AP cell, thus special windows are necessary for specific light transmission of the light source energies. Currently, there several options exist for cell windows on the reaction cell: i) a borosilicate window, which has a transmission of more than 90% between 350-2500 nm; ii) a sapphire window, which is useful in a transmission range of 330-5500 nm; iii) a fused quartz window, which is a more suitable material choice for UV light; iv) any other window material in the correct size which satisfies the needs of the users' experiment. User supplied light sources can also be attached to the main chamber with minimal effort.

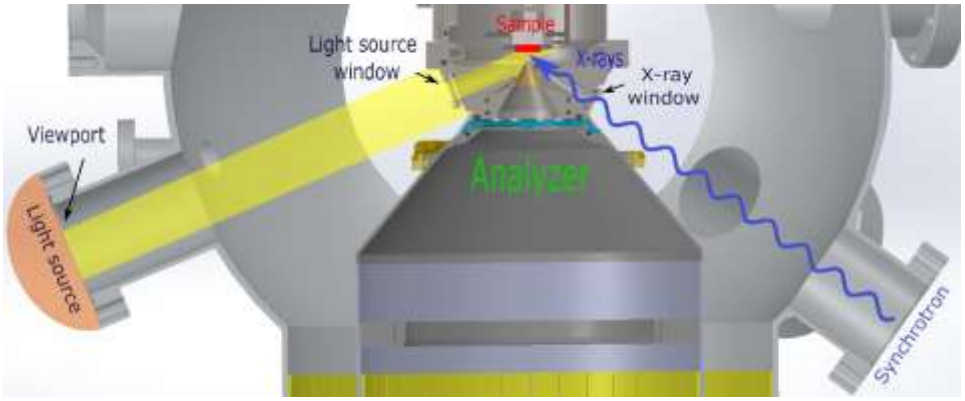


Figure 7. Layout (top to bottom view) of the alignment between the external light sources, the synchrotron radiation and the analyzer nozzle in the analysis chamber with AP cell.

### 2.3.3 Ambient pressure cells

Several ambient pressure cells are available for users depending on the experimental needs. They all consist of the manipulator assembly, the "cell chamber" (the UHV chamber where the cell is initially placed and that can be separated from the analysis chamber via a gate valve), and the gas system. The manipulator allows for the motion of the cell in x, y, and z directions in order to move the cell into the analysis chamber and dock it with the lens of the analyzer along with lateral sample movement. Once the cell is docked and fixed in place, the sample inside can be moved forwards with its own dedicated motor mounted on the sample holding shaft.

In each cell, the sample can be heated. The sample heaters are based on a resistively heated element which is placed just under the sample so that heat is efficiently conducted and radiated to the back of the sample. Additionally, a special heater assembly is available which also houses a cooling loop that can be used to cool samples below room temperature using either cold liquid (alcohol-water mixture) or cold $N_2$ gas. In all cases,

the sample temperate is measured using a K-type (Alumel-Chromel) thermocouple typically spot welded on the sample or on the sample plate.

The synchrotron radiation enters the AP cell through a very thin (200 nm) X-ray window (Figure 7~~Figure 7~~). The window material can be selected between $Si_3N_4$, Al, or Zr, depending on which material's transmission curve best suits the experimental needs. Typically, the Al window is used in almost all experiments, because it offers the best compromise between giving a high flux at high and low energies. The Al window only has a very low transmission between 70 and 200 eV, however since the beamline has the best flux at these energies, it is still very much possible to conduct experiments using these energies. Figure 8~~Figure 8~~ shows the transmission of the various windows.

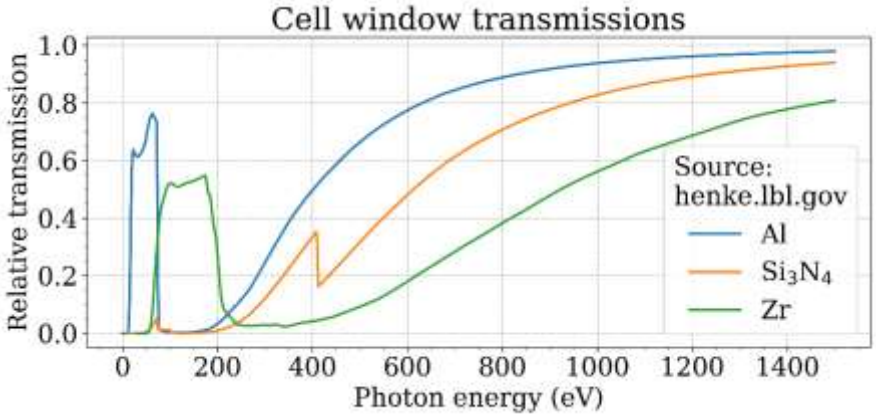


Figure 8: Transmission of the X-rays through 200 nm of Al, $Si_3N_4$, and Zr. Data is taken from the Center for X-ray optics. [5]

The cells can be operated in many different gas flow modes. The outlet line of the cell is equipped with a variable opening valve, which can be directly controlled by a capacitance gauge installed next to it. Through a hardware feedback system, a pressure setpoint can be defined, allowing the variable opening valve to be controlled automatically to achieve the desired pressure. This mode of operation is useful if the actual flow through the cell is unimportant, but a specific pressure is desired instead. However, the capacitance gauge is located quite far from the actual sample area, and therefore the pressure reading could differ. The capacitance gauge, while being gas independent, is only sensitive to pressures above ~0.1 mbar, and therefore a combined Pirani and cold cathode gauge is also located on the outlet line to be able to estimate the pressure in the cell over a wide range from 1 bar to $3\times10^{-6}$ mbar. The cell outlet is typically pumped with a turbomolecular pump, but in high-flow scenarios, the pump can be bypassed so that the forevacuum system handles the gas load instead.

The AP cell gas composition is controlled through a gas manifold system which is equipped with a combination of mass flow controllers and variable leak-valves. Both gases and vapors (*i.e.* $H_2O$, EtOH, etc.) can be introduced. The mass flow controllers also allow for quick switching of the gas. Additionally, mass spectrometry of the reactant gases can be performed using a quadrupole mass spectrometer (QMS) (used primarily on the outlet line of the AP cell with the possibility of probing gas on the inlet line as well) or using a time-of-flight mass spectrometer (TOFMS) located in the pre-lens section of the electron analyzer. The QMS has higher mass resolution, and it analyses the gas composition of the outlet/inlet line while the TOFMS probes the gas composition that enters the pre-lens chamber directly above the sample surface. Both mass spectrometers can run simultaneously during XPS acquisition, allowing correlation of changes in reactant gas composition to changes seen on the surface.

[5] B. L. Henke, *et al.*, Atomic Data and Nuclear Data Tables **54**, 181 (1993). Website.

**Standard cell**

The cell used for the majority of the experiments (including catalysis, redox studies, etc., essentially everything except thin-film growth research) is called the "standard" or catalysis cell. The cell is unique in the way the gases are introduced into the cell. There are two independent gas inlets, which on the air side contain separate gas introduction systems consisting of leak-valves and mass flow controllers. The gas tubes combine at the front of the cell, where they are directed towards the sample using the so-called "double cone" setup (Figure 9~~Figure 9~~). The double cone setup consists of the original cone with an aperture of about 0.3 mm in diameter where the photoelectrons pass through and are collected in the analyzer. Surrounding this cone is a larger cone with an aperture of about 3 mm in diameter. The gas is introduced into the cell between the inner and outer cones. Gas flow simulations indicate that this configuration allows the incoming gas, by geometry, to pass near the sample. This increases the chance of interactions with the surface and decreases the amount of unreacted gas that bypasses the sample completely (a scenario that could happen in a setup where the pumping tube is located right next to the inlet).

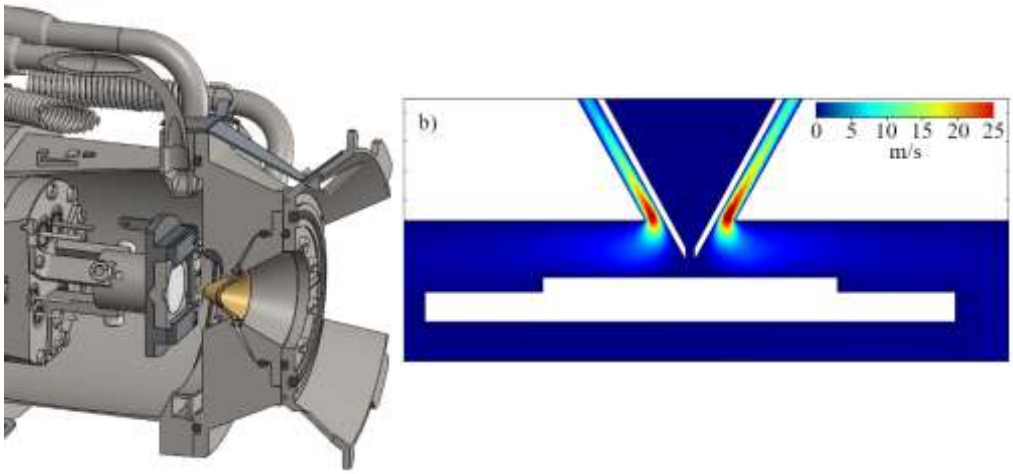


Figure 9. A 3D model of the standard cell showing the sample stage and the double cone inlet system (left). Gas flow simulations in a simplified cell model show how the gas enters just above the sample (right). The simulation shows the velocity magnitude of the gas in units of m/s.

The catalysis cell is based on the original AP cell designed in 2012[6,7], but it has been significantly improved. The most significant change is the addition of the double-cone system and a resistive heater. The standard cell was designed in collaboration with Synchrotron SOLEIL, MAX IV Laboratory, and Lund University.

The original version of the cell heater design consisted of a Pt filament in an alumina enclosure. However, due to the predominant catalytic activity of a hot Pt filament exposed to the same catalytic conditions as the sample, mass spectroscopy results of the reaction products from model catalysts and single crystals studies were very challenging to interpret or sometimes completely useless. The heater was therefore changed to a commercially available pyrolytic boron nitride/pyrolytic graphite (PBN/PG) heating element from Thermic Edge. The PBN/PG heater has the advantage of being catalytically inert while reaching the desired temperatures in nearly all experiments with high pressures as was achievable in the Pt filament-based heater. The PBN/PG heaters are, however, extremely sensitive to oxygen and hydrogen atmospheres. When heated in these environments, the graphite layer gets thinner, and the heater and power supply lose contact very easily. Since the heating system causes the majority (90+%) of the technical issues faced during beamtimes due to the need for elevated temperatures (up to 600 °C, depending on environment) in the standard cell, we believe that a different kind of heating system is essential to improve the reliability under typical reaction

[6] J. Knudsen, *et al*. Surf. Sci., 646, 160–169 (2016).
[7] J. Schnadt, *et al*. J. Synchr. Rad., 19, 701–704. (2012).

conditions. The new system is already in the planning stage, as detailed later in this document (see section 5.2).

**ALD cell**

The ALD cell is a dedicated sample environment for atomic layer deposition and other *in situ* thin-film growth studies. All experiments that employ difficult-to-use ALD precursor gases use the ALD cell, which minimizes the risk of cross-contamination with experiments requiring cleaner conditions (*e.g.* the standard cell). The ALD cell differs from the standard cell in the way the gases are let into the system. The cell has two independent gas inlets which are directed towards the sample surface. Opposite the gas inlets is a pumping tube connection, which should facilitate a laminar-like flow over the substrate surface. The two gas inlets are separated to prevent undesired deposition in the gas tubes themselves. To avoid condensation of precursors, the inlet gas tubes and cell walls are wrapped with a resistive heating element allowing to heat the tubes and walls to moderate temperatures (~100 °C). The substrate itself can be heated using a Pt filament-based button heater underneath the sample. The maximum temperature of the substrate is limited to about 400 °C, due to the lack of cooling capability in the cell. A schematic model of the ALD cell is shown in Figure 10~~Figure 10~~.

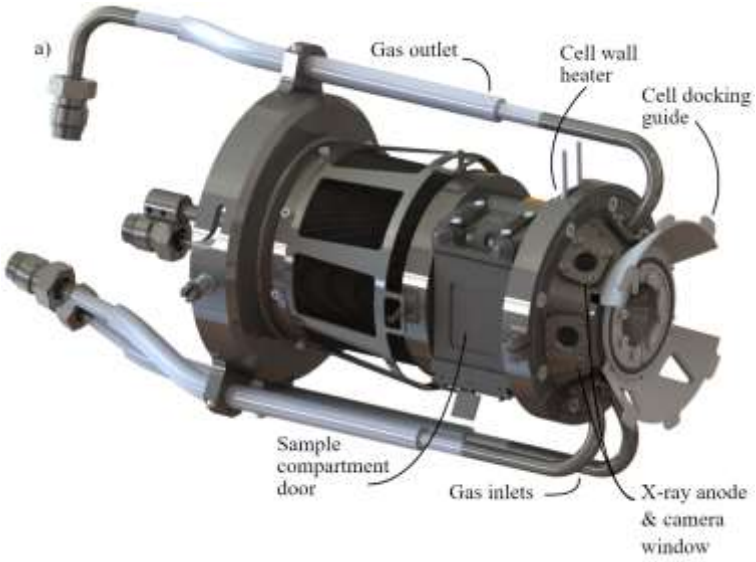


Figure 10. 3D model of the ALD cell showing some of the most important components.

Many different types of ALD precursors have been used in the cell, a selection of which is detailed in Table 1~~Table 1~~. The cell was designed for versatility with the use of a wide variety of ALD precursors. The gas tubing can be changed according to the specific needs of the experiment. The most common experiments deal with a two-precursor process which consists of a metal-containing precursor and an oxygen-containing precursor as the co-reactant. In these cases, the beamline offers a well-tested setup where users can directly attach their own precursor with minimal changes. Due to safety requirements most precursors should come in deposition system bottles which are easy to install on the system with no risk of harm to personnel around the beamline area. The gas system consists of pneumatically operated valves which can be remotely controlled using a pulsing control system. A pulse scheme can be programmed in, allowing one to automate the dosage of many ALD cycles.

Table 1: A list of commonly studied ALD reactions and their respective precursors. The list is not exhaustive, only indicative of the common conditions.

| Film | $HfO_2$ | $TiO_2$ | | | Cu | | Pt |
|---|---|---|---|---|---|---|---|
| **Metal precursor** | TDMAHf | TTIP | TDMAT | $TiCl_4$ | $Cu(dmap)_2$ | $Cu(hfac)_2$ | $MeCpPtMe_3$ |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **One of the used co-reactants** | $H_2O$<br>Ozone**<br>*hυ** | $H_2O$<br>*hυ** | $H_2O$ | Isopropanol | *hυ**<br>$ZnEt_2$ | $H_2O$ | $O_2$ |

*Xe lamp light source (Hamamatsu L6605), which is available to all users.
**Ozone delivery system is under commissioning and not yet available to general users.

### 2.3.4 Ambient pressure electron energy analyzer

The main instrument of the APXPS endstation is the Phoibos 150 NAP electron energy analyzer from SPECS GmbH. The analyzer features a special connection on the lens system, on which the AP cell can be docked using a bayonet-like coupling mechanism. The analyzer consists of a differentially pumped lens system with four turbomolecular pumps in total. This, together with the small cone (diameter of 300 µm) of the AP cells, allows pressures of up to 20 mbar in the cell with the detector remaining at an operational pressure. Most of the gas is also removed by the first pumping section (known as the pre-lens) which decreases the electron scattering losses further in the analyzer.

The analyzer is equipped with a delay line detector (DLD). The DLD consists of a microchannel plate array for pulse amplification and an in-vacuum readout unit consisting of meander structured delay line wires (DLD anode). Each hit position is encoded by a fast data acquisition unit, which may also detect the hit time referenced to an external clock. DLDs are single counting devices; therefore, the complete device works linearly even at extremely low numbers of incoming electrons. The detection principle limits the maximum detectable count rates at least due to the maximum delay of the meanders. The maximum count rate in the fourfold coincidence measurement can be up to $2 \times 10^6$ counts per second without saturation.

The most commonly used analyzer mode is fixed analyzer transmission (FAT) mode for XPS acquisition. The FAT mode scans through electron kinetic energy while holding the pass energy constant, thus ensuring constant energy resolution throughout the scan. The retarding potential of the analyzer is varied to measure different electron kinetic energies.

For fast data acquisition, a snapshot mode is available. In this mode, the analyzer voltages are not scanned, instead data is collected from all channels of the detector simultaneously without performing any averaging. The spectrum shows the energy distribution of the electrons that pass through the analyzer with its current settings (*e.g.* pass energy). Snapshot mode allows for fast data acquisition over a limited energy range, dictated by analyzer settings, compared to FAT. Snapshot measurements are well-suited for DLDs, which have hundreds of channels allowing high energy resolution and timing capabilities. Nevertheless, the snapshot mode requires careful detector calibration in order to remove any possible detection inhomogeneities on the microchannel plates (MCPs).

The DLD measures all events in temporal reference to an external clock. For this external reference mode, the user needs to start the time-to-digital-converter (TDC) by an external clock. Time measurements are performed by summing up the arrival times of pulses at the end of the DLD meander, i.e. the same results which are used to determine positions for each event are summed.

In general, the DLD can be operated in three different modes, all of which can be considered to be within the "time-resolved XPS" category. These modes are:

- Unsynchronized measurements: No signals are used for synchronization. Instead, the data is expected to be highly repeatable and therefore allows the use of event-averaging or Fourier transformation techniques with a periodic structure within the data. This kind of data acquisition scheme is exemplified for example in the measurements by J. Knudsen et al[8].
- Intermediate resolution time-synchronization: An external digital signal (TTL) can be supplied as an internal reference start signal. This allows synchronization of the acquired data from upwards of 1

[8] J. Knudsen et al., Nat Commun **12**, 6117 (2021).

ms without any practical upper limit. Such synchronization makes it possible to synchronize to relatively slow perturbation schemes, for example with gas pulses. This was demonstrated in work by Redekop et al[9].

- High time-resolution synchronization: Using the direct synchronization port on the TDC, it is also possible to use a TTL level signal to reference the detector electrons to an external signal. This clock is capable of reaching close to the ultimate timing resolution of the FPGA (about 100 ps), but it is practically limited to about 20 µs long acquisition schemes. Therefore, it is in practice only capable of resolving very fast perturbation schemes. One such example is synchronizing the detection to the ring clock from the 1.5 GeV storage ring as shown in Figure 11~~Figure 11~~.

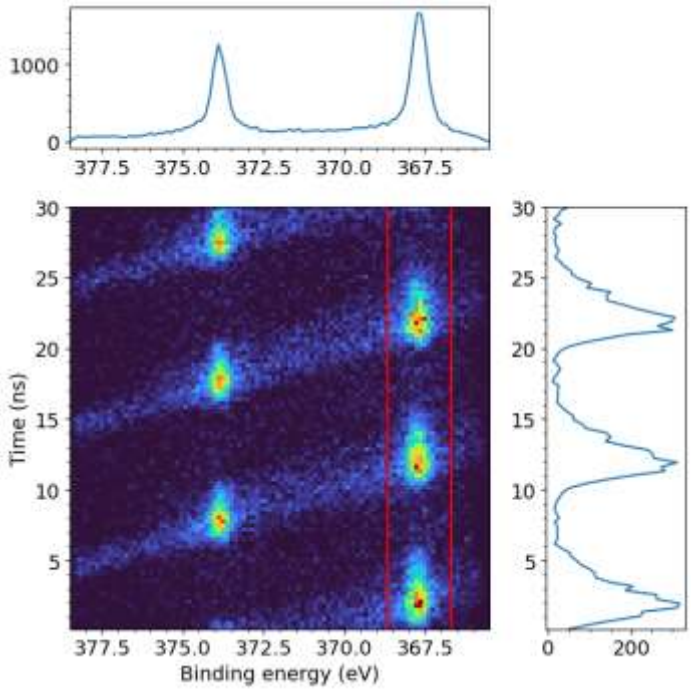


Figure 11: Example of time-resolved data synchronized to the 1.5 GeV storage ring clock. The graph shows results from the measurements of an Ag crystal in the Ag 3d region detected from individual light pulses which are separated in time by 10 ns. The data is tilted in time due to the different kinetic energy of the electrons. The counts inside the red lines are summed up in the rightmost panel.

### 2.3.5 Gas system

The main gas system for the APXPS endstation is, at the time of writing this report, still under construction. Since regular user operation began during early 2020, the endstation has used a temporary gas system which is modified depending on the needs of each experiment. Typically, it has consisted of 2-3 mass flow controllers and 1-2 variable leak-valves, shown in Figure 12~~Figure 12~~. The use of hazardous gases requires that the gas bottles be placed in ventilated enclosures. Therefore, the total number of gases installed at the same time is usually 3-4, of which only two may be hazardous. Using the leak-valves, it is also possible to dose liquids or solids which have high enough vapor pressure.

Only MAX IV staff and beamline staff are allowed to connect and disconnect gas bottles to the gas system. Users are allowed and are encouraged to use the gas system once the bottles are installed. Users are given a brief introduction to the gas system, especially regarding the placement of various valves in the system that they will use in their experiment.

[9] E. A. Redekop et al., Review of Scientific Instruments **92**, 044101 (2021).

Typical flows through the MFCs are less than 10 mL/min when the gas is used for the experimental reaction inside the AP cells. This results in typical pressures of a few mbar inside the AP cell. When bottles are installed and lines need to be flushed clean, much higher flows can be temporarily used.

The APXPS endstation has an interlock system that is designed to prevent an accidental release of gas into the cell beyond the approved pressure limits. Pressures are constantly monitored by gauges in the outlet line of the AP cells (high pressure side), pre-lens of the analyzer and on the UHV side of the chamber (low pressure side). If higher than anticipated pressure is detected, the interlock system is triggered and valves are closed on the inlet lines towards the AP cell, preventing any further increase of gas in the cell or analyzer. Additionally, the mass flow controllers are turned off so that no further gas is let in. The same interlock system also disables the voltages on the analyzer and closes the beamline valve when high pressures are detected.

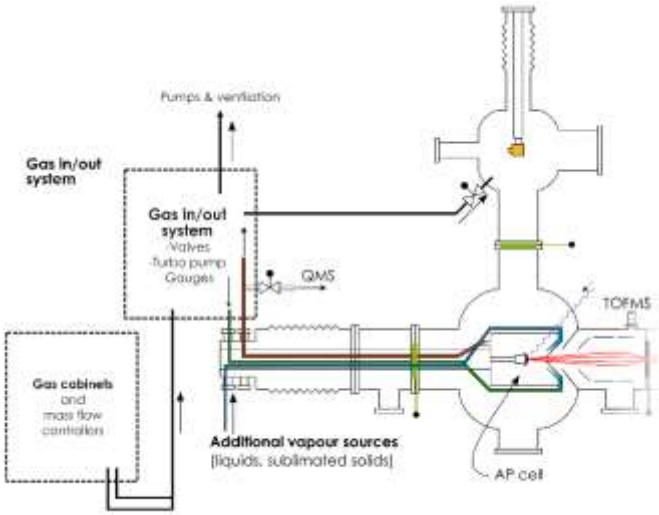


Figure 12: The layout of the temporary gas system installed at the APXPS endstation. The schematic shows the location of the temporary gas cabinets with respect to the rest of the gas system.

## 2.4 Endstation B (RIXS endstation)

The RIXS endstation (see Figure 13~~Figure 13~~) has two spectrometers covering the wide energy range from 30 to 1000 eV. It supports measurements on various kinds of samples ranging from solids to liquids and gas-phase, and studies related to the molecular structure of liquid water, mixtures, and solutions can be addressed. Furthermore, RIXS spectroscopy can be used to investigate cycling effects on the electronic structure of electrodes in Li-ion battery electrodes as well as of corrosion processes of transition metals. The endstation also provides a NEXAFS detector and a manipulator with high precision sample scanning capability.

The endstation consists of four highly customized chambers: The upper chamber serves as a load lock chamber where new samples can be loaded, the bottom chamber where the synchrotron radiation meets the sample, and the two spectrometers in their own separate chambers. All the chambers can be isolated from each other using gate valves, making maintenance and other such works easier to perform.

Two RIXS spectrometers on the endstation are the GRACE, a wide range, moderate resolution spectrometer, and the plane grating spectrometer (PGS), which is a low energy, high resolution spectrometer with very high transmission. The spectrometers are mounted perpendicularly with respect to the incoming photon beam and opposite to each other.

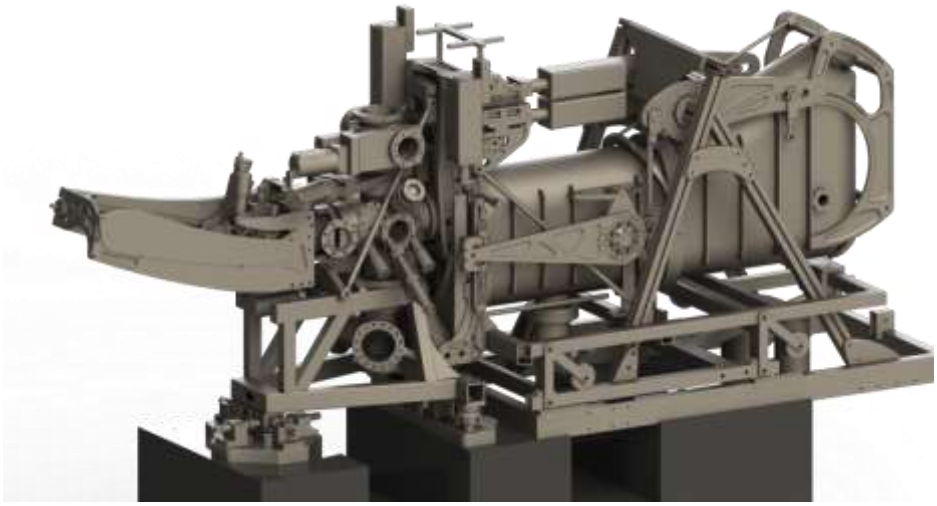

Figure 13: Overview of the RIXS endstation as seen from the beamline direction with the PGS instrument on the right and the GRACE instrument on the left.

### 2.4.1 GRACE spectrometer

The GRACE spectrometer[10] is a modified Scienta XES320 which is operated in a slitless mode. The spectrometer houses three spherical gratings with line densities of 300 lines/mm (3m radius), 400 lines/mm (5m radius), and 1200 lines/mm (5m radius). When the spectrometer is operated in the first or second diffraction order, it can cover the photon energy range of 50 to 1500 eV at a reasonable resolving power. Typically, the accessible energy range is limited to about 650 eV (for Mn L-edge) and below which gives resolving power in the hundreds to about 2000. An example result is shown in Figure 14~~Figure 14~~.

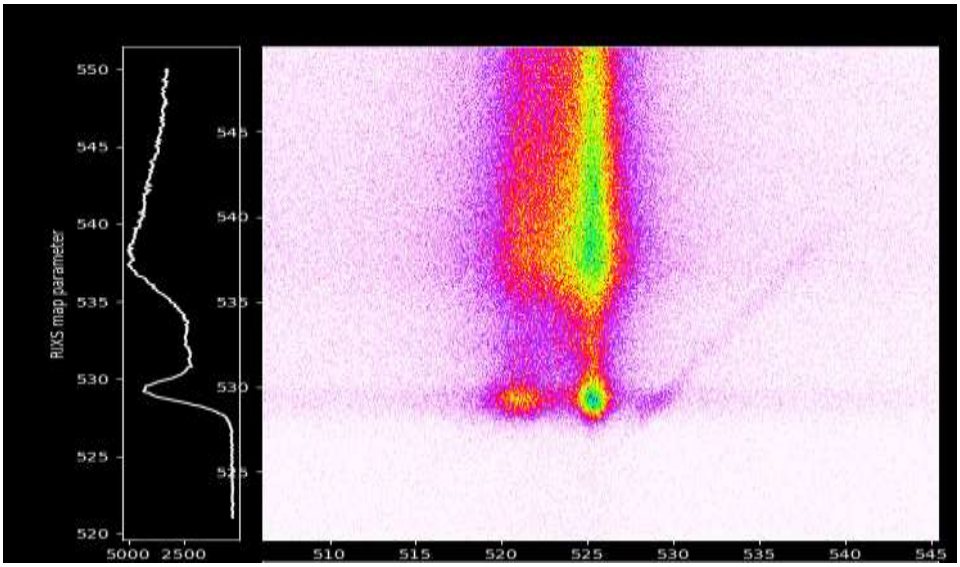


Figure 14: An example RIXS map from Kapton foil measured over the O K-edge with the GRACE instrument.

[10] J. Nordgren, *et al.*, Rev. Sci. Instrum. 60, 1690 (1989).

### 2.4.2 Plane grating spectrometer (PGS)

The PGS[11] consists of a collimating parabolic mirror, a large 1200 lines/mm grating, and a final plane parabolic mirror which focuses the diffracted light into the detector. This kind of optical scheme yields a high throughput and good energy resolution (10-30 meV) in the range of 27 to 200 eV.

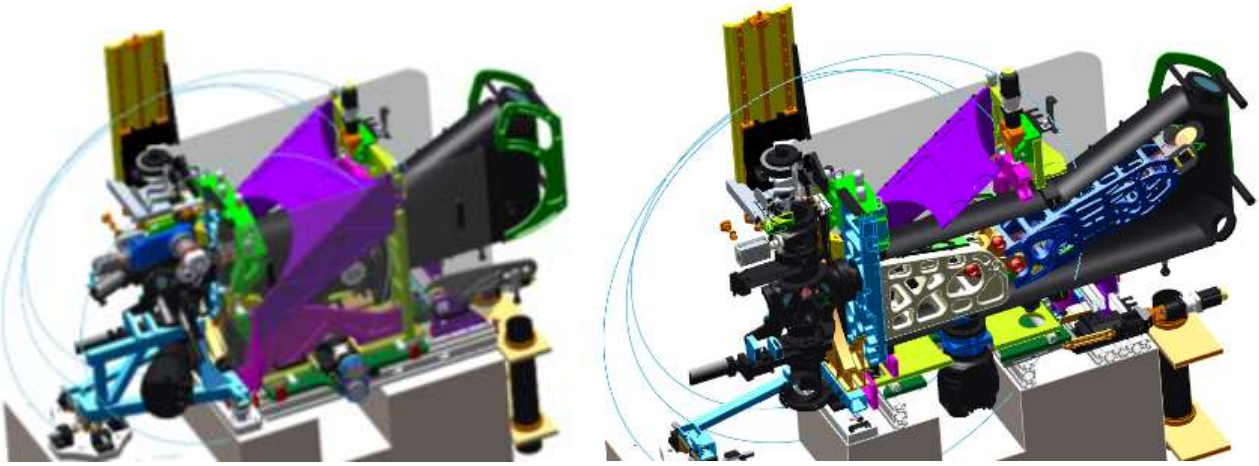

Figure 15: Left: The alignment mechanics of the PGS instrument. Right: View of the optics inside the chamber and internal mechanisms.

The instrument saw a major overhaul to its mechanical design when it was adapted to SPECIES beamline. The most important adaptations were changes to align with MAX IV motion system standards (encoders and stepper motors). The possibility to align the instrument along the beam to the best available focus position from the M4 mirror was added to increase the versatility of the instruments. At the time of writing this document, the instrument was in late commissioning phase and first users are planned for spring 2024.

### 2.4.3 Detector readout and data acquisition software

All RIXS instruments at MAX IV currently use MCP based detectors with delay-line anodes (DLDs) for readout. Since there are no available commercial RIXS instruments or data acquisition (DAQ) solutions on the market this means that efforts have had to be spent on developing the RIXS software tools needed for both the SPECIES and the Veritas beamlines. A lot of this development and testing has been conducted at the SPECIES RIXS endstation. As of April 2024, a new data streamer protocol has been deployed to ensure stability and sustainability of this software developed jointly by the beamline staff and the MAX IV scientific computing group. This streamer separates the DAQ from the software control interface (GUI) that is needed to view and manipulate the data. The data format for each RIXS event contains the X and Y positions and the timestamp. This has the advantage that the experiment can be fully recreated after the measurement ensuring that no data is lost even if the measurement control software loses contact. This is important since acquisition times for all RIXS are often quite long.

A GUI for viewing and calibrating the data has been developed and is currently in use on both SPECIES-RIXS and at Veritas. A standalone version of the program has also been compiled and can be offered to users for post-production of the spectra from the raw data.

To maximize the signal-to-noise ratio of the measured RIXS spectra, the DLD can be synchronized to the bunch clock of the storage ring. The time resolution of the synchronization is dictated by the data acquisition electronics and is about 100 ps. This method is known as time gating and allows discarding all the signals that are generated when there are no light pulses hitting the sample.

[11] M. Agåker, *et al.*, Nucl. Instrum. Methods Phys. Res., Sect. A, 601, 213 (2009).

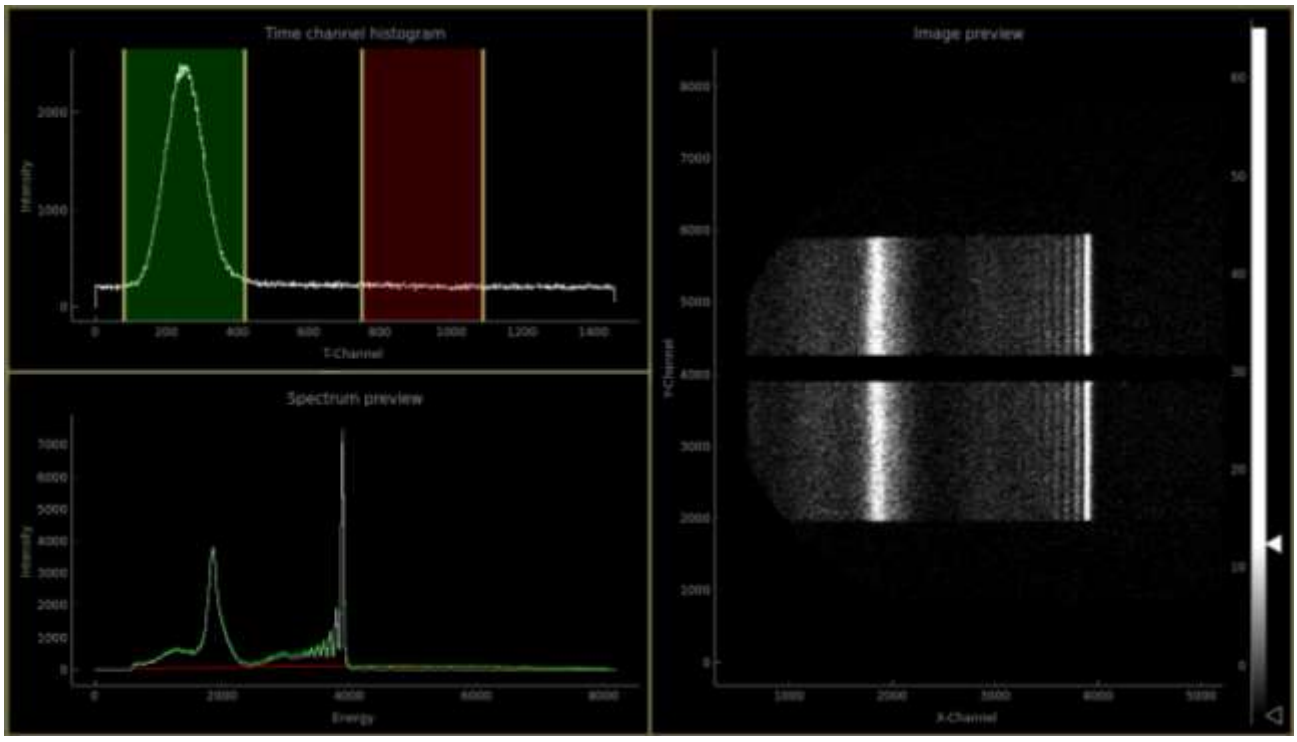


Figure 16: An example of a time gating window set to coincide with the light pulse from the storage ring (green area on the top panel and the green curve on the bottom panel). A second identical window is set in between the light pulses (red area on the top panel and red curve on the bottom panel) and is used as dark count image to improve the signal-to-noise ratio.

Another time stamp can also be introduced into the data, which can be used to monitor changes on longer timescales from µs and up. This is useful when monitoring sample damage over longer term (see Figure 17~~Figure 17~~). It can also be used to investigate long term interference such as energy drifts of the incoming photons over time.

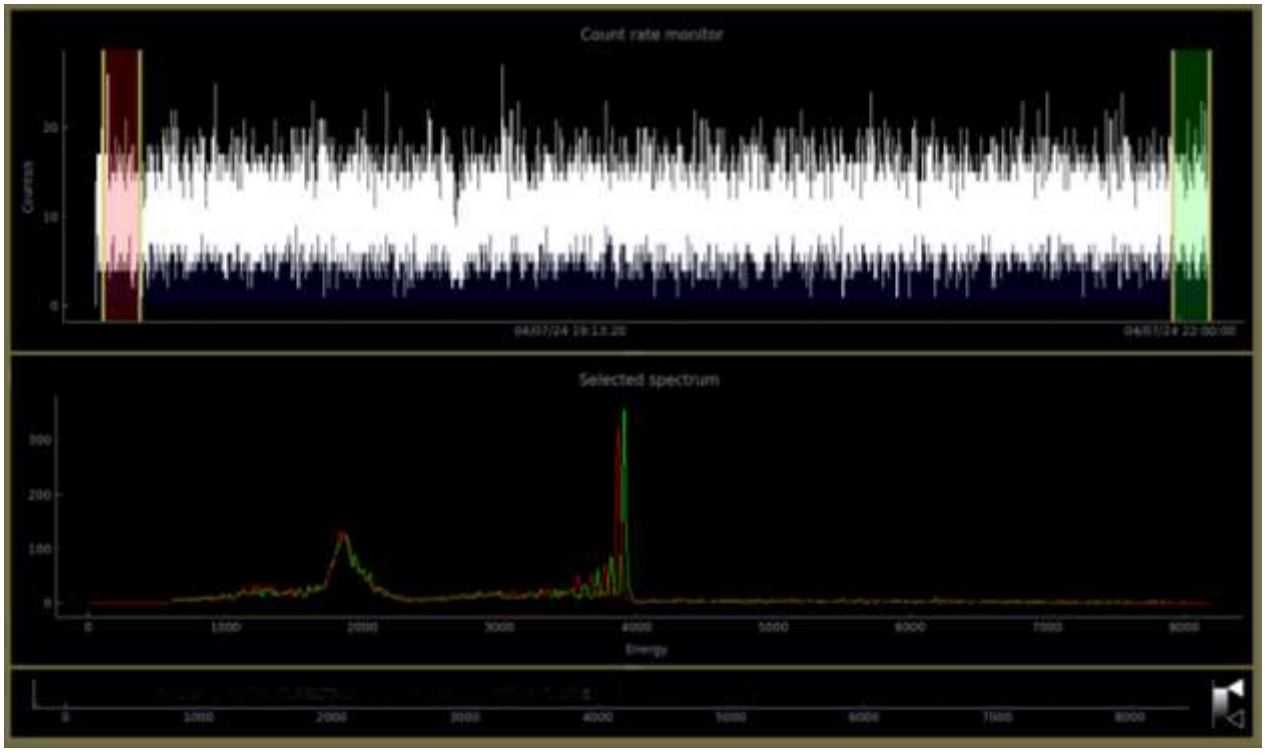


Figure 17: RIXS data plotted over time. The bottom panel shows the same spectrum measured before and after a several hour exposure.

In addition, tools have been developed to greatly improve the on-the-fly handling of the generated RIXS data. For example, a curvature can be set to the recorded 2D data, which can be used to set the emitted energy scale. Several datasets can be plotted at the same time for easy visualization and RIXS maps can be easily generated. All raw data is streamed directly from the detector to an HDF5 file. The same format is used by the user interface where the raw data is again saved with all calibrations and the resulting spectra and RIXS maps are added.

### 2.4.4 RIXS high stability sample manipulator

As the development of the SPECIES RIXS endstation coincided with the design phase of the Veritas RIXS endstation, the need for RIXS to have a very stable sample manipulation system with a high degree of versatility and accuracy was identified. This challenge could therefore be more efficiently tackled jointly. No commercial solutions meeting the high needs with a reasonable price were identified. Therefore, a new manipulator (shown in Figure 18~~Figure 18~~) was developed as part of the two projects on the two beamlines[12].

Figure 18: The RIXS manipulator design enabling 200 nm accuracy and repeatability of the samples and showing no eigenfrequencies below 40 Hz is a prerequisite for sample scanning, spot size measurement and being able to measure samples down to a micrometer scale.

The manipulator is an essential part of any operations at the RIXS endstations and has also found its way outside of MAX IV (for example to European XFEL and Sirius). An important part of setting up and executing all experiments is to align the sample to the beamline focus position. Stable sample manipulation capabilities are also essential in order to mitigate sample damage in the beam. Another software tool was developed for spatially mapping samples and setting up sample scanning very easily. This tool also keeps track of what parts of the sample have been exposed to X-rays during the measurements.

[12] M. Agåker, *et al.*, J Synchrotron Rad 28, 1059 (2021).

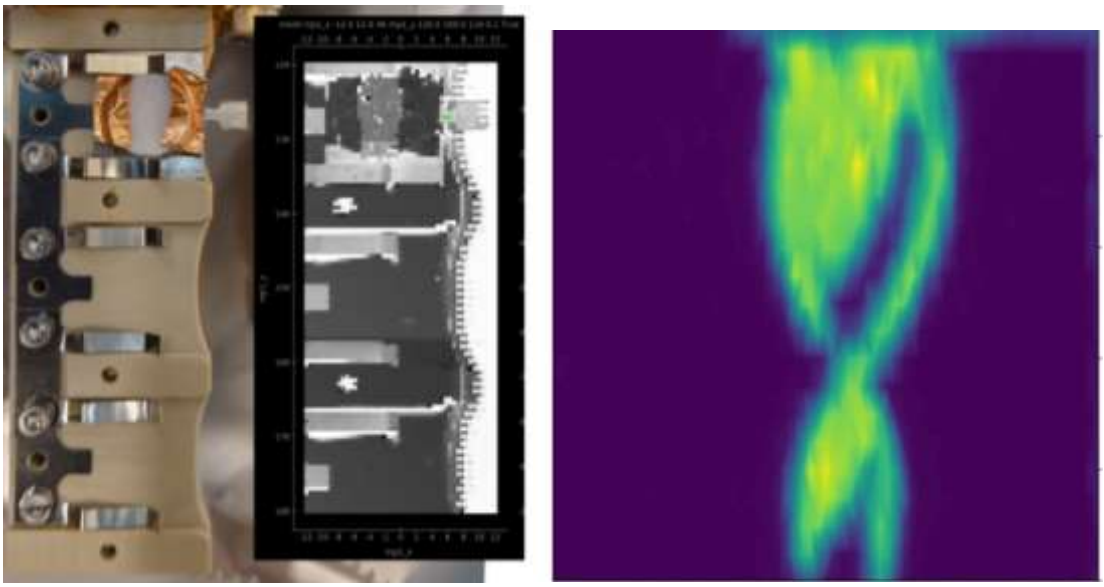

Figure 19: Left: The sample stage in one of the sample rods with three sample slots. The right side shows a sample scan made with the sample tracker which easily identifies the sample due to its different contrast. Right: sample scan of a flowing liquid jet (flat jet) measurement.

### 2.4.5 RIXS sample environments

The goal for both RIXS beamlines is to offer RIXS opportunities to a broad range of users. This means the sample environments have to cater to needs ranging from high vacuum requirements for condensed matter physics users to liquid jets. The endstation and spectrometers are designed with this versatility in mind offering load-lock options compatible with custom made Argon glove-box setup, in-vacuum suitcase sample transfer to filter valves protecting optics in both spectrometers and beamline. A differentially pumped inner chamber is designed to be inserted to further separate the sample environment from the surrounding vacuum systems. The actual sample environments are designed as rods that are mounted from the top through the manipulator that provides a basic 4-axis manipulation to align the samples to the incoming X-rays and to the spectrometers. There is also the option to mount an X-ray absorption detector that can be set up for total fluorescence yield (TFY). For some sample environments total electron yield (TEY) can also be measured through sample drain current.

An initial set of sample environments has been developed jointly by MAX IV and Uppsala University financed from three main funding sources: The initial Wallenberg grant for Veritas, the transfer package budget from VR and an SFF grant held by Marcus Agåker at Uppsala University. All sample environments have the option of adding the focus finder and multilayer reference sample, for optimizing sample positions in the beam and measuring reference data, respectively. Table 2~~Table 2~~ shows the sample environments available at SPECIES. In addition to the listed ones, a fully motorized 6-axis cryo manipulator rod will also be available for RIXS experiments from 2025. New sample environment developments are under discussion with the user community.

Table 2: List of sample environments currently offered to users at SPECIES-RIXS and Veritas. Some have not yet been used at SPECIES due to low demand and might require additional changes to the main chamber layout.

| Sample environment | Description | XAS | Notes |
|---|---|---|---|
| **6 slot rod** | 3 omicron slots for LN2 cooling.<br>3 insulated omicron slots | TFY and TEY | |
| **5-axis cryo head** | 1 omicron slot with in-vacuum manual azimuthal adjustment | TFY and TEY | Closed cycle He-cryo compatible |

| | | | |
|---|---|---|---|
| **Low temperature cryo head** | 1 omicron slot with added shielding for sub 10 K temperatures | TFY | Close cycle He-cryo needed. |
| **Flow cell** | Multipurpose flow cell. Can be run with either membranes or pinhole | TFY | Gas-phase and liquids possible. |
| **Liquid jet** | Both round jet and flat jet. | TFY | A He sheet version is under development for liquids with high vapor pressure. |

## 2.5 Experimental infrastructure

Most of the beamline infrastructure was described above. Here we provide information on important upcoming experimental infrastructure installations and all the supporting facilities available in the lab.

### 2.5.1 APXPS endstation

One of the most important infrastructures for the APXPS endstation is the new gas delivery system, which we will briefly describe here.

The new gas system consists of three gas cabinets, two enclosed gas panels and one cabinet for gas sensing detectors. Each gas cabinet consists of four gas lines. The twelve gas lines are connected to the two gas panels. Each gas cabinet and gas panel are connected to the ventilation system. The gas safety system will be implemented in a centralized safety PLC that is constantly monitoring the gas composition in the ventilation system. In case any hazardous gas is detected at a larger than expected amount, the necessary precautions are taken (i.e. the valves in the gas system are closed and appropriate alarms raised).

The gas line starts with the bottle and a gas regulator (shown schematically in Figure 20~~Figure 20~~). A gas flow orifice is installed after the regulator. The orifice improves safety in the case of regulator malfunction by limiting the maximum gas flow. The regulator is then connected to a 3-way valve. This makes it possible to connect two different bottles (with their own regulators) to the same gas line. Each gas line is connected to a nitrogen line which makes it possible to purge the gas line when gas bottles need to be exchanged. Each line also contains a pressure transmitter (for monitoring the absolute pressure in the line) and some safety functions to relieve too high pressures (these include a burst disc and a pressure relief valve, in series). The burst disc breaks if there is a failure of the regulator and high-pressure gas enters the pipe system. In such a case, the gas is evacuated through the evacuation line. If such an incident were to occur, the necessary alarms are raised in the nearby areas to notify any people present. The last component of the gas line before the gas panel is the pneumatic gas valve. This valve will close in a number of scenarios, including a detected leakage, that the doors are left open too long, or that the ventilation is below the minimum.

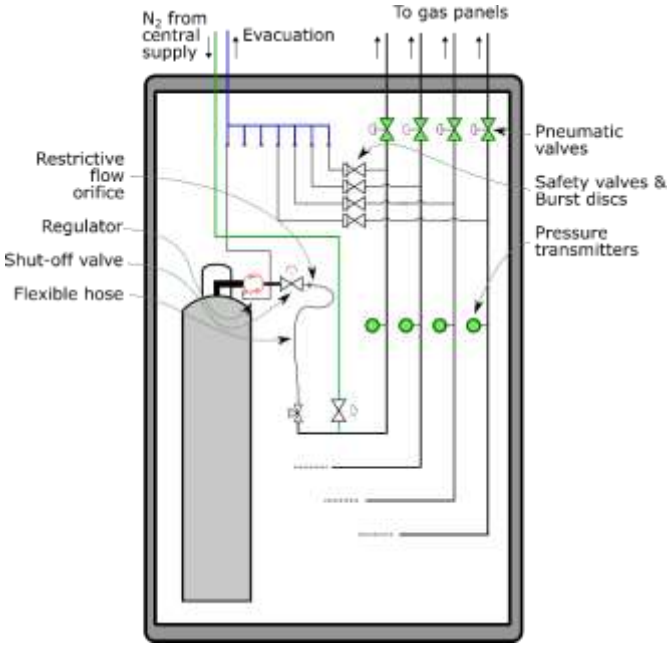


Figure 20. Schematic view of one of the gas cabinets housing the gas bottles.

The gas mixing panels are designed for precise and controlled dosing of gases into the AP cell. The system consists of multiple couplings, filters, valves, and MFCs placed inside the gas panel enclosure. Currently, in the two gas panels, there are several inlets for feeding the gas into the gas dosing panels. Figure 21~~Figure 21~~ shows the possible connections between the gas cabinets and the mixing panels. The gas dosing panel has one outlet to provide gas supply to the AP cell. The maximum pressure inside the gas lines is restricted to 2.5 bar before the MFCs and 20 mbar after them. There are two gas dosing panels. One panel is dedicated for oxidizing and flammable gases ($O_2$, $H_2$, CO, etc.) and is intended to be used with the standard and ALD cells. The second gas mixing panel is intended for sulfur-containing gases ($H_2S$, etc.) and will be used with the proposed sulfur cell. The reason for separating sulfur containing gases into its own gas mixing panel is to minimize cross-contamination. The vacuum systems on both panels are nearly identical. The gas dosing panels are bakeable, which is necessary for eliminating impurities from the gas lines.

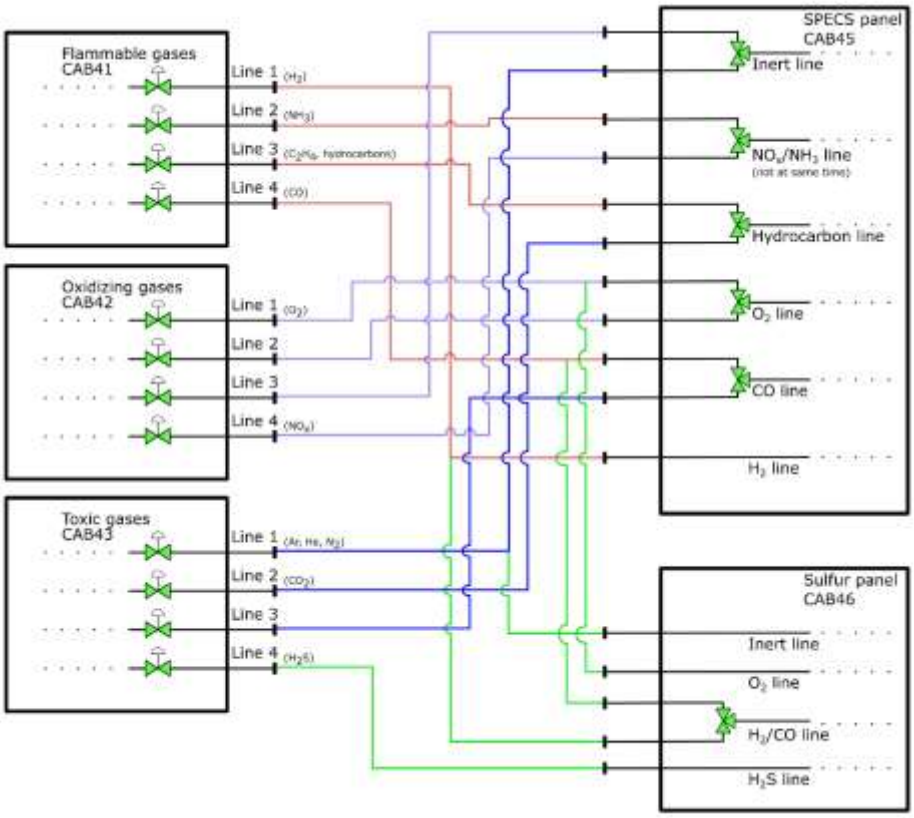


Figure 21. The connections between the three different gas cabinets and the two gas mixing panels. The complexity of the system is intended to increase the usefulness of the gas system for a broad range of experiments.

### 2.5.2 RIXS

As covered earlier, the RIXS endstation is built to be versatile and offer RIXS and NEXAFS opportunities to a wide range of users. Currently this means that the infrastructure besides the normal media installations is light but for the future some gas installation similar to the APXPS branch might be needed. A close cycle He-cryo is missing at the moment, one is currently installed at Veritas but complicated to move due to the need of a compressor unit.

### 2.5.3 Common and shared facilities

SPECIES users have access to various shared facilities at MAX IV. These include chemical laboratories (fume hoods, glove boxes, any sample preparation requiring chemicals), the sample preparation lab (optical microscopy, some light sample treatment), and the microscopy laboratories (SPM lab). Most users need to use some of the facilities in their sample treatment and MAX IV has established a common pathway to request access and receive the necessary safety training.

In addition, MAX IV offers help via the “sample environments and detectors” (SEDS) support group who host a number of instruments that can be temporarily borrowed for experiments. The borrowed instruments typically range from power supplies to light consumables. A common instrument SPECIES often borrows is a chiller unit often used to connect to the sample cooling line in order to cool samples to below room temperature. The achievable temperature is around +5 °C which is required for achieving high relative humidity with water vapor in the cell. In addition, SPECIES receives support from the detector specialists working in SEDS who support on-going development and maintenance efforts on detectors and MCP units.

The beamline users also have access to various instruments built for transferring samples around the facility in a manner that they are not exposed to air. In case samples need in-vacuum transfer, a vacuum suitcase from the microscopy laboratories can be borrowed. This is typically needed when moving sensitive samples between the beamline endstation vacuum chamber and the SPM lab vacuum chambers. The beamline has

also built an “atmosphere suitcase” which is a small, enclosed, vacuum chamber that can hold static vacuum or be filled with inert gas and taken inside the glove boxes in the chemical laboratories. This is useful if air sensitive samples need to be pre-treated inside the glove box and transferred to the beamline under inert atmosphere.

# 3 Beamline operation

SPECIES was in operation for a short time in the old MAX IV facility on the MAX II storage ring. Several successful user experiments were conducted, which have also been reported in about 25 publications. Here, however, we will focus on the work done after the beamline was transferred to the 1.5 GeV ring in the new MAX IV facility. The beamline received first light on April 1st, 2019, and after a brief commissioning period, it welcomed the first expert user group during the autumn of 2019 and began regular user operation in March 2020. Initially, users were only at the APXPS branch, as it was ready before the RIXS branch was able to offer regular user operation. On the RIXS branch regular users were welcomed from 2021 onwards.

Beamtime distribution follows MAX IV recommended guidelines on the APXPS branch. Approximately 75 % of beamtime is made available to general users, while the remaining 25 % is for maintenance, commissioning, and in-house research. On the RIXS endstation, the portion of general user operation is slightly less due to the need for more endstation commissioning activities.

Beamtime is split between the two branches so that about 60 % of the time is dedicated to the APXPS branch and the rest for RIXS. The staff at each branch decide on user operation and in-house activities independently, but it is ensured that user operation is given about 75 % of the total time available at the beamline.

MAX IV issues regular proposal calls for granting experiments at beamlines. There are two open calls per year, except during 2021, when the calls were merged due to issues related to the pandemic. To assist in the allocation of beamtime, several MAX IV Programme Advisory Committees (PAC) have been appointed. The committee reviews and evaluates submitted proposals and provides recommendations for the allocation of beamtime, based on the scientific excellence and feasibility of the suggested experiments.

## 3.1 Modes of operation and statistics

**Standard access:** The so-called standard beamtimes at SPECIES are typically 30 to 36 shifts long (24 hours = 6 shifts) or 5 to 6 days, depending on the accelerator delivery calendar (currently the first Tuesday of each month is reserved for beamline commissioning activities and are not part of deliverable beamtime). Occasionally shorter beamtimes are granted, typically 18 shifts. Shorter beamtimes require careful planning, pairing experiments together to minimize time spent re-configuring the endstation between experiments.

**Fast access:** In 2022, SPECIES began to offer the so-called fast access mode to all users. This mode is continuously accepting users with the idea being that users would be able to gain access for quick measurements with only a short delay from proposal submission to the actual experiment. A maximum of 6 shifts (1 day) are offered per user in this scheme. Fast access mode consists of two different categories: technical feasibility intended for quickly testing new samples or new environments that a user is uncertain of its success or a scientific experiment which is intended for completing one or more datasets that have missing spectra in an otherwise complete dataset for publication.

During autumn 2023 and spring 2024, the fast access mode was temporarily discontinued. For the next cycle, it is planned to reinstate the fast access mode.

**Industrial access:** SPECIES has had two industrial beamtimes from a company focusing on the production of position sensitive photodiodes and testing their products in a real synchrotron beamtime.

In each call, the beamline is open to offering more industrial beamtime should the need arise.

**Training and education:** There have been no requests from external users. Only the beamline staff have used training and education beamtime during the Spectroscopy Summer School in 2023.

**In-house:** In-house beamtime is distributed by beamline staff to various aspects of beamline development, which can be divided into the following categories:

- Beamline commissioning: Beamtime used for testing and characterizing beam parameters and ensuring stable beam qualities. The beamtime is also used for testing new instruments, or endstation capabilities. In the beginning of beamline operation, commissioning beamtime was used extensively, but it is steadily decreasing to a stable level determined by the new development needs. Some small amount of beamtime is used to periodically check beamline performance.
- In-house research: Scientific research conducted by the beamline staff.
- Invited users: In some cases, users can be invited to the beamline to carry out their research in collaboration with the beamline staff. This kind of in-house time is usually strategically targeted to a specific development activity which requires testing and modifying to bring new capabilities online. If there is a need to expand the user community, the beamline staff can also invite potential new users to the beamline to carry out initial experiments in hopes of establishing a new regular user group. This is particularly useful when reaching out to establish new areas of scientific research.

In addition to the modes listed above, there are often cases where beamtime becomes available outside of typical beamtime availability. On the 1.5 GeV ring, this happens quite regularly with the so-called single-bunch mode operation of the ring. This beamtime is not offered on the regular call for normal users at SPECIES due to the much lower flux available. However, the beam can be used for preliminary studies (especially in UHV conditions) for future proposals or in some cases for fast access proposals. This time is considered “bonus” time for the users and is not included in the beamtime availability calculations.

### 3.1.1 Proposal statistics

The beamline team keeps track of all experiments using an Excel sheet where the beamline staff (usually the local contact) logs the experiments and adds information on the successes, failures, publications, etc. Various aspects can be analyzed from simple proposal statistics to the “success” of experiments. SPECIES was included for the first time in the autumn 2019 call and began user operation in March 2020 with just the APXPS endstation offering beamtime to the users initially. Below, we show a selection of the statistics gathered over the past 4 years of regular user operation.

Figure 22~~Figure 22~~ shows the total number of finished shifts since the start of user operation. In 2020, the operation was dominated by in-house activities since several sample environments and other capabilities were still being commissioned. Just under 50% of shifts were made available for general users during 2020 (Figure 22~~Figure 22~~). Subsequent cycles have seen a steady increase in the total number of standard (PAC) shifts, which is due to the decrease in used in-house beamtime. It is important to note that Figure 22~~Figure 22~~ does not include shifts used for beamline or endstation commissioning. Since the RIXS endstation has used a lot of beamtime for commissioning, the figures disproportionately indicate more beamtime usage for APXPS.

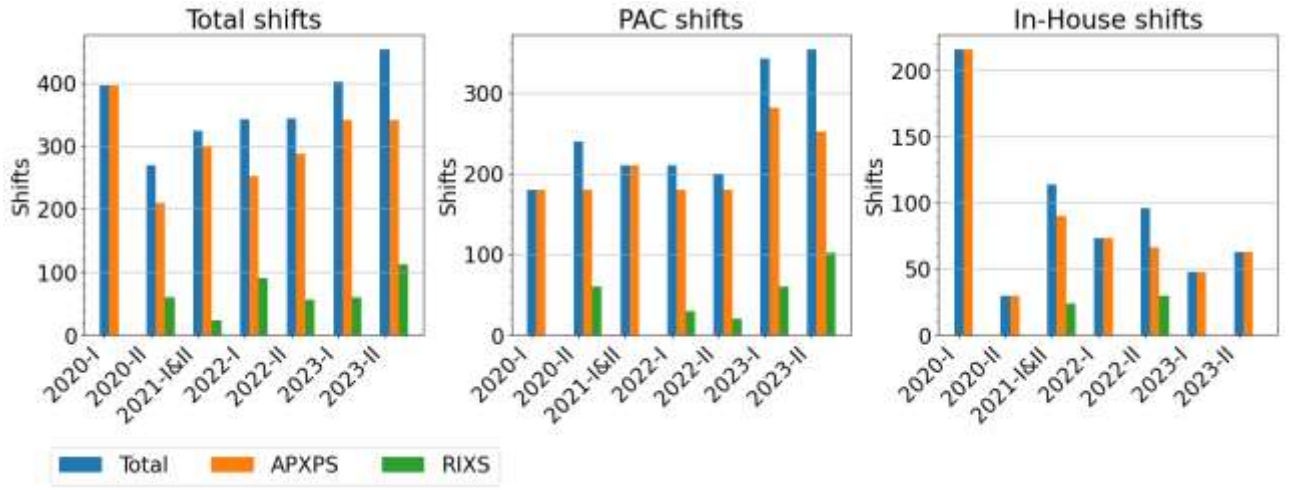


Figure 22: Total number of finished shifts in each proposal cycle since the start of the user programme in early 2020.

It is also interesting to compare the submitted and accepted proposals in order to be able to calculate the oversubscription numbers. Figure 23~~Figure 23~~ shows the submitted and finished proposals for all the proposal cycles including the oversubscription number. The variation in the oversubscription factor is quite high from cycle-to-cycle. This is likely caused by several effects, most notably, the availability of various sample environments which vary between cycles. The RIXS endstation was offered for the first time in the 2020-II call with the exception of the special 2021-I&II call (which was special due to the pandemic). A small number of proposals can also be transferred between SPECIES, HIPPIE, and Veritas. This is typically 1-2 per cycle but has not been accounted for in the data displayed in Figure 23~~Figure 23~~

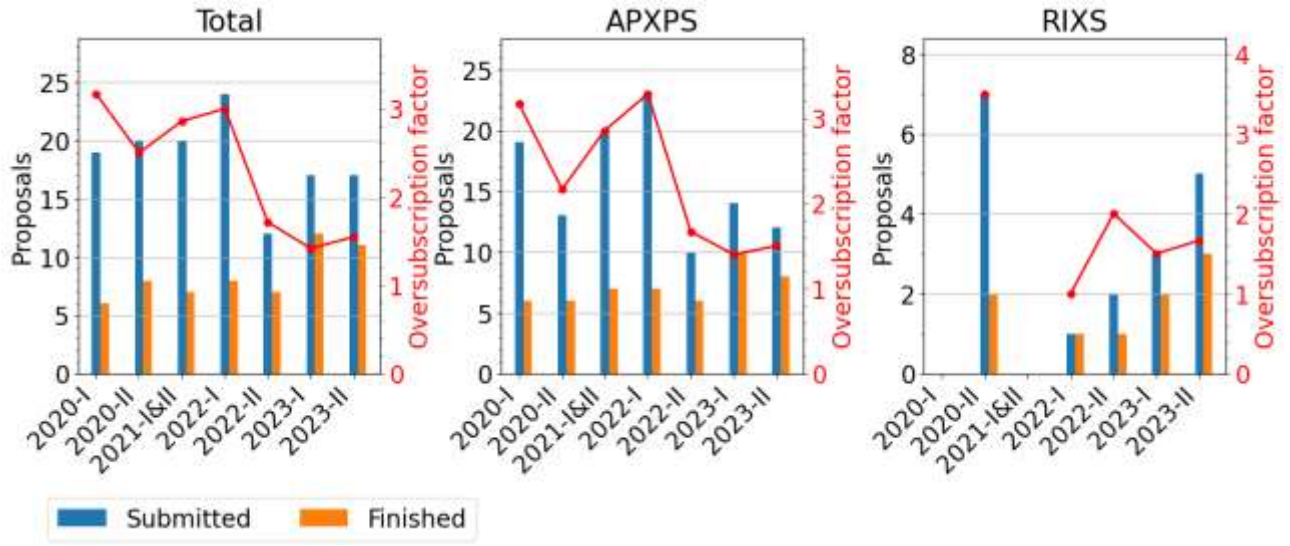


Figure 23: Submitted and finished proposals for the total beamline and for both branches individually. Oversubscription numbers are plotted on the red curve on the right axis.

We can also investigate the geographic origin of the userbase shown in Figure 24~~Figure 24~~. Sweden has the largest fraction of users nearly always. The user distribution shown in Figure 24~~Figure 24~~ follow the overall trends observed across MAX IV beamlines.

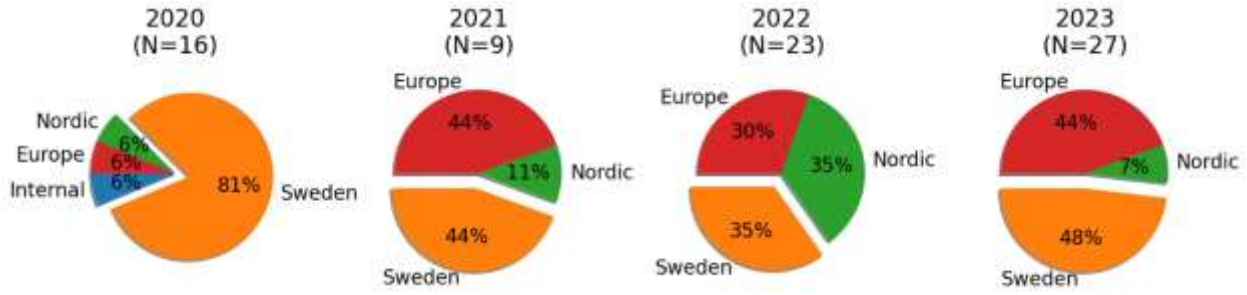


Figure 24. Userbase country of origin for the past four years where N represents the number of user groups.

It is also interesting to see the use of the ALD cell in the proposal distribution, since its introduction to the regular user operation starting in 2021 at the APXPS endstation. This is plotted in Figure 25~~Figure 25~~, where it is evident that the ALD cell proposals increased in the first three cycles and reached a relatively stable level, comprised of approximately 40-50% of all completed proposals. It is encouraging to see that usage of the ALD and the catalysis cells has been approximately equal for three proposal cycles. This fact is reflected in the submitted proposal breakdown between the two cells as well. For example, in the most recent call ("Spring24"), both the ALD cell and catalysis cell received five proposals each, and four proposals were granted time on each cell. The division of proposals both submitted and awarded was therefore 50 % for the Spring24 cycle. Note that this calculation does not reflect upon the likelihood of awarded beamtime for either cell, since all proposals are strictly reviewed on scientific merit without pre-defined beamtime allocation for either cell.

The average length of an experiment using the standard cell has decreased due increased use of fast access (typically experiments lasting < 3 days) with this cell, therefore it is informative to also compare the number of delivered shifts for each cell, in the most recent cycle this number is approximately equal. The "other" category is all experiments which do not use either of the cells (often referring to UHV studies). These are rarely PAC granted proposals, but instead originate from users who have used additional, i.e. "bonus", beamtime for example during single-bunch days or weeks.

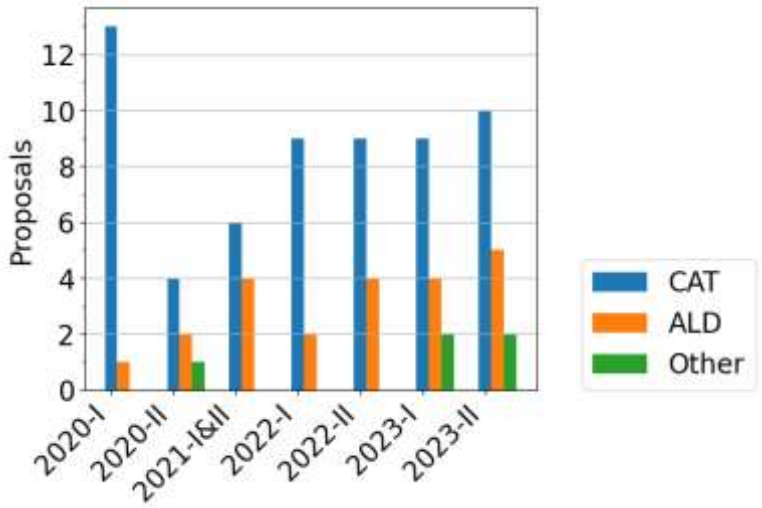


Figure 25: Completed proposals in each cycle for the various cells at the APXPS endstation where CAT refers to the standard or catalysis cell, ALD refers to the ALD cell, and "Other" represents experiments that did not utilize either cell.

We have also analyzed new vs. returning users for each cycle as presented in Figure 26~~Figure 26~~. Among returning users, we isolated Swedish users (blue) from other users (orange). The data from finished experiments was processed by assigning each user to a specific user group and if that user group returns with a new proposal (even with a different PI) they are counted as a returning user. The trends indicate that the Swedish user community is more likely to return than international users.

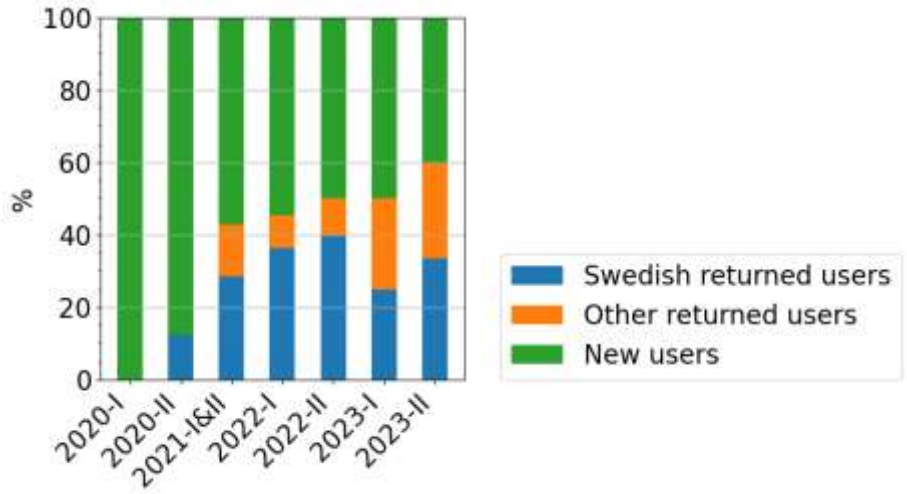


Figure 26: Trends of new and returning users, distinguishing Swedish from international return users. A returning user is defined as a user group that has performed an experiment at SPECIES.

## 3.2 Staffing

The beamline is operated by two teams: the APXPS team (led by Andrey Shavorskiy) and the RIXS team (led by Conny Såthe). The APXPS operates three instruments across the SPECIES and HIPPIE beamlines. On the HIPPIE beamline these instruments include a solid-gas endstation dedicated to general purpose APXPS and a solid-liquid endstation dedicated to mostly combined electrochemistry and APXPS experiments. The team members work closely with each other so that most staff are well versed in all techniques across multiple beamlines. In-house beamtime is also frequently considered to be a team effort where the staff participate in each other's experiments. However, user support is often provided by the team members that are permanently based at the beamline where the experiment is occurring.

The RIXS team runs day-to-day work at the Veritas beamline. All members of the team are, however, well versed with the SPECIES-RIXS endstation and give regular user support there. The interaction between the beamlines is very natural as the RIXS instruments have several common technological aspects (sample environments, detectors, acquisition schemes, etc.) that are nearly interchangeable between the two beamlines.

The team structure is visualized in Figure 27~~Figure 27~~.

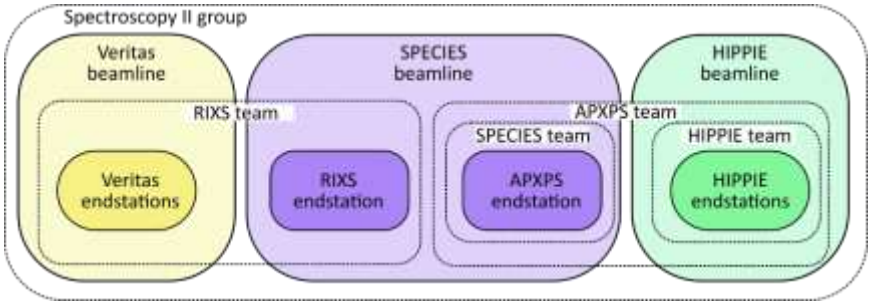


Figure 27: Interfaces between the various teams and their main placements within the three beamlines.

The APXPS staff at SPECIES consist of:

- Esko Kokkonen (beamline scientist)
- Alexander Klyushin (beamline scientist)
- Margit Andersson (beamline engineer, <70% working time)
- Calley Eads (Postdoc until 08/2024)

- Mihai Pop (software engineer, 33%)
- Rosemary Jones (Postdoc at LU, 20%)
- Joachim Schnadt[13] (Prof. at LU, 20%)

The APXPS members listed above also have the responsibility of day-to-day operations at the beamline. They ensure good beam quality and carry out periodic maintenance tasks at the beamline. The rest of the APXPS team consists of personnel at the HIPPIE beamline.

The RIXS team consists of:

- Conny Såthe (beamline scientist)
- Takashi Tokushima (beamline scientist)
- Anirudha Ghosh (beamline engineer)
- *Vacant* (beamline postdoc)
- Marcus Agåker (Scientist at UU, 25%)

This team shares their work between the SPECIES-RIXS endstation and the Veritas beamline.

In addition, MAX IV central resources have people who are not associated with the beamline but who act as single points of contact towards the rest of the organization. Most of the technical assistance towards the beamline comes from the technical division including software, electronics, and engineering groups. The most frequent collaboration lies within the software group, where there is a dedicated contact person at SPECIES with whom weekly meetings are organized and on-going tasks are discussed. The other groups (for example, engineering groups) are contacted on an as-needed basis, most often through the ticket system.

## 3.3 Typical beamtime process

A beamtime at SPECIES is normally one week long, typically starting on Tuesday or Wednesday mornings, depending on the machine schedule. During the initial scheduling, each experiment is assigned a local contact whose primary role is to ensure smooth running of the experiment before and during the beamtime. One month before the beamtime, the local contact gets in touch with the users and asks them to carry out all the necessary experimental and safety forms including creating the experimental session in the digital user office (DUO). The typical beamtime process and its involvement of the various resource groups is highlighted in Figure 28~~Figure 28~~.

The previous experiment often ends on Monday mornings. The rest of Monday is spent exchanging samples and gases and baking the system to achieve a good base pressure for the next experiment. However, because of the division between RIXS and APXPS weeks, it is rare to have consecutive experiments scheduled on the same branch. Therefore, there is typically plenty of time to exchange the user setup from one experiment to the next.

The users are encouraged to arrive early at the beamline to prepare their samples and set up any external instruments they may need to use during the beamtime. Thus, making the best use of their beamtime by beginning their measurements as soon as the beam is available. On the RIXS branch, the beamline staff often aligns the samples to the beam ensuring proper signal is read on the spectrometers. The local contact assigned to the experiment gives all the necessary instructions for smooth operation of the endstation and provides general safety guidance plus additional safety instructions if the experimental safety classification demands it. The local contact stays in close contact with the users the first few days so the users have the possibility to readily ask any questions. The aim of this process is to leave the users feeling comfortable

[13] Recently appointed as the interim science director of MAX IV

operating the instrument independently throughout the nights and weekends for efficient and effective use of the beam.

The local contact supports the users during office hours (8-17) and afterwards with an on-call service until 23:00 on weekdays. On weekends, the on-call service spans twelve hours from 08:00 until 20:00. During this time, the local contact should be reachable by phone and be able to assist the users with issues, particularly if the problem stalls the experiment completely. If the problem cannot be resolved on the phone, the local contact may attempt to resolve the problem remotely or return to the lab. The local contact receives a base level monetary compensation for the on-call work and additional compensation for any work that requires remote intervention or coming back to the lab.

Since 2022, MAX IV has offered a 24/7 support service in the form of “floor coordinators” dedicated to supporting all operations in the lab. SPECIES users are encouraged to contact the floor coordinators whenever they first encounter issues. While the floor coordinators are not experts at the beamline and might not be able to solve more complex issues, they have been trained to solve simple problems at the beamline. Floor coordinators can also help contact the correct person, where possible, to solve problems outside of local contact working or on-call hours.

The support given by the local contact varies depending on the needs of a user group. If the user group is experienced, then only technical support is needed. Often some scientific questions can also be discussed. In cases where the local contact is a collaborator of the user group, it is natural to be much more involved with the entire process, including supporting the users with scientific analysis of the data. Such cases are in the purview of the local contact and the group manager. Depending on the level of support given by the local contact, the users are encouraged to involve them in the capacity of co-author in any forthcoming manuscripts.

After the experiment, the local contact performs a quick informal interview with the users before they leave the lab to obtain information on the success of the experiment and the impression of the beamtime. This information is later used by the beamline team to evaluate overall progress and success of all experiments. The local contact also informs the users on any pending tasks, such as data storage and retrieval, metadata, etc., that could be useful in the data analysis process.

After about six months to one year, the beamline team will be in contact with the users to inquire about the status of the data evaluation, ask whether anything is missing that could be amended with additional (possibly fast access) experiments, and the possibility of a manuscript.

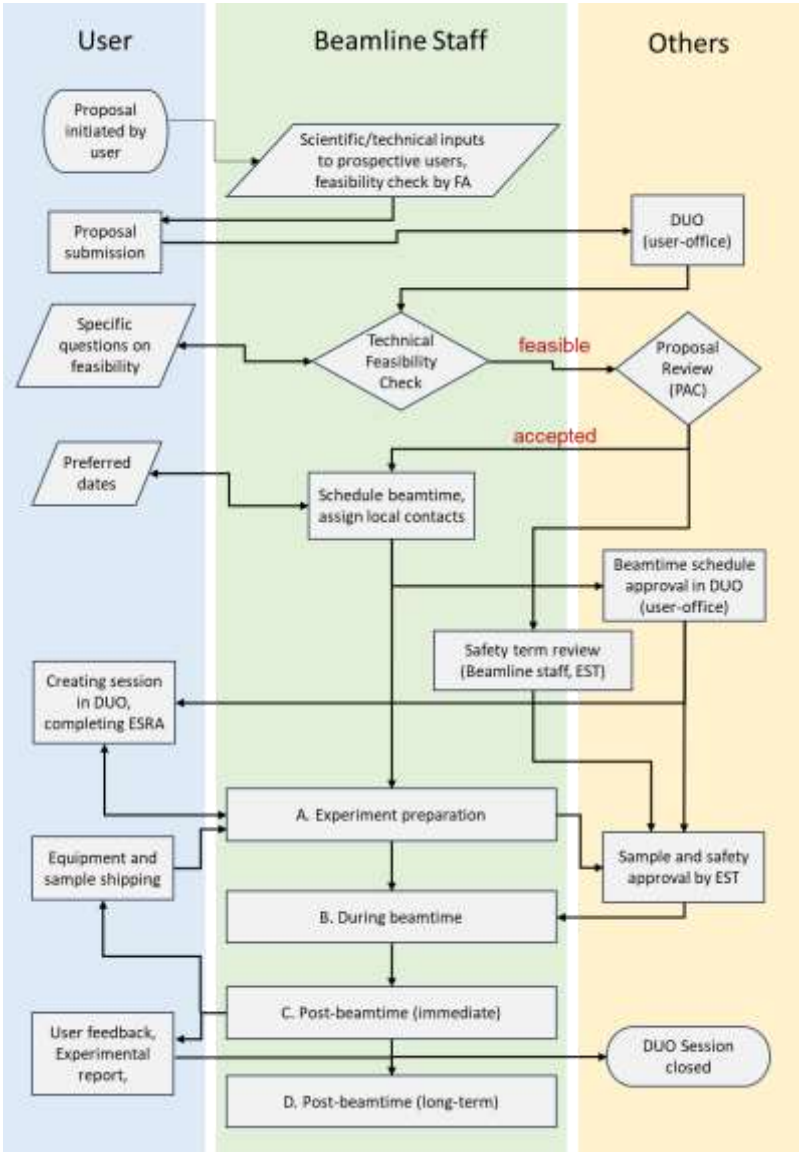


Figure 28: Typical beamtime process involves several steps with users, beamline staff, and MAX IV support functions. Abbreviations used here are DUO: Digital User Office, PAC: Programme Advisory Committee, EST: Experimental Safety Team, ESRA: Experimental Safety Risk Assessment. Picture: M. Ramakrishnan, Figure 72, Balder beamline MAX IV beamline review report.

## 3.4 Community outreach

The beamline team reaches out to the community in several ways:

**Regular email updates.** Prior to the closing of each proposal call, the APXPS team sends out a short newsletter informing the users about the upcoming call deadline including endstation capabilities. The newsletter also includes information on beamline updates and other important news from the HIPPIE and SPECIES-APXPS beamlines. The newsletter reaches about 500 email addresses.

**Conferences.** The APXPS group attends several international conferences, where either the entire beamlines are presented, or some specific scientific or technical project is highlighted. Some of the most important conferences are: The APXPS workshop (annual), the ALD conference (annual), Synchrotron Radiation Instrumentation SRI (every three years). The APXPS team was involved in organizing the APXPS workshop in Lund in 2019.

The team is naturally heavily involved in the MAX IV User meeting, organized annually. In the most recent user meeting, a special APXPS mini workshop was organized with a good attendance (approximately 40 people, in person and online).

**MAX IV outreach.** The team participates in regular outreach activities organized together with MAX IV communications team and other beamlines. Such as, the collaborative effort to increase knowledge of MAX IV capabilities at Swedish universities through a MAX IV "roadshow" organized during 2020-2021. Also, the communications team at MAX IV regularly releases news stories about the science done at MAX IV, including results from users' experiments at SPECIES.

**Summer school.** During August 2023, the first 'Spectroscopy Summer School' was organized at MAX IV, as part of that event some practical exercises were carried out on both branches. The summer school was aimed towards PhD students and recent postdocs who might apply for beamtime at a MAX IV spectroscopy beamline. Staff at SPECIES were involved in the organization and funding of this summer school.

**Other activities.** SPECIES will participate in the PRISMAS programme over the next 4-5 years. PRISMAS is a doctoral training programme funded together with EUs COFUND action, which is part of the Marie Skłodowska-Curie Actions Programme. The PRISMAS programme includes a secondment to the participating beamlines at MAX IV for PhD students. SPECIES is part of 3 PRISMAS projects, listed below, the PhD students will be co-supervised by beamline staff and are expected to apply for beamtimes together with their supervisors throughout their PhD. During their secondments to MAX IV, they will also contribute to the development and operation of the endstation through various small projects. The projects at SPECIES include:

- *Stroboscopic operando spectroscopy of the dynamics in atomic layer deposition by event-averaging: experiment and theory* (Supervisor: Prof. Joachim Schnadt, Lund University; co-supervisor: Dr Esko Kokkonen)
- *Chlorine Surface Activation Mechanism on Wildfire Smoke Particles and Its Relevance to Stratospheric Ozone Depletion* (Supervisor: Dr Xiangrui Kong, Gothenburg University; co-supervisor: Dr Alexander Klyushin)
- *Quantum properties of direct-Chemical vapor Deposited two-dimensional (2D) heterostructures* (Supervisor: Associate Prof. Venkata Kamalakar Mutta, Uppsala University; co-supervisor Dr Anirudha Ghosh)

## 3.5 Funding acquisition

The SPECIES team seeks external funding whenever opportunities arise. Some larger external funding opportunities include:

- High-temperature cell (Crafoord grant, 2023), 2 MSEK (~ 180 k€)
- External light sources for ALD experiments (Crafoord grant, 2021) 100 kSEK (~ 9000 €)
- ALD cell (Academy of Finland, together with Helsinki Univ., 2017), 200 k€
- Beamline Transfer package (VR, 2014), 13 MSEK (~1.1 M€)
- Research Infrastructure Fellow (SSF, Marcus Agåker, 2015), 15 MSEK (~1.3 M€)

Several funding schemes have been realized in collaboration with the Finnish privileged access programme (FIMAX). FIMAX is a consortium of Finnish universities and research organizations who contribute to MAX IV operations with funding and other support. In return, they can receive guaranteed access time at any MAX IV beamline. Through FIMAX, several projects at SPECIES are fully or partially funded and smaller equipment has been purchased. These include:

- Solar simulator
- Funding of the ALD cell (as specified above)
- Partial funding of the upcoming high-temperature cell (specified later in section 5.2)

At the time of writing this document, there are several funding applications under review. These include an application to Crafoord foundation for a gas chromatograph (detailed more in section 5.2) and several funding applications for postdoctoral positions that would be shared between MAX IV and other universities (discussions on-going with researchers from Lund University and University of Oslo, for example).

## 3.6 Project management

The various on-going projects at the beamline can be categorized into different groups depending on their urgency, scope, and need for centralized MAX IV resources. For small things required to maintain a stable level of operational readiness, the beamline has access to short-term resources within MAX IV that can be booked with minimal bureaucracy (for example, through a ticket system or simply by approaching the appropriate persons). In addition, some resource groups provide a single point of contact at the beamline. One such example being the software group as discussed previously. The beamline meets with the software group contact person every week to discuss the status of on-going tasks and decide task prioritization.

For tasks of intermediate size that require more resources from MAX IV, a centralized project management structure exists. The beamline can submit a project at any time to the "Beamline Programme Advisory Group" (BPAG), which handles all incoming projects from the beamlines and assigns them resources according to the need and availability. BPAG projects are relatively small and are funded through the normal beamline operational budget.

For large tasks, the project should be submitted to the "Central Project Office" (CPO), where a trained project manager is often assigned to the project to oversee its completion with a reasonable timetable and to act as an interface between the resource groups and the beamline staff. CPO projects are typically externally funded and require the coordination of several MAX IV resource groups. Some CPO projects also span several beamlines, which highlights the need to have an external project manager who can focus on the project as a whole and coordinate between beamlines.

SPECIES currently has several ongoing BPAG and CPO projects, which are explained in detail in section 5.

## 3.7 User feedback

Beyond the informal discussion with beamline staff directly after a beamtime has ended, DUO prompts each user for feedback with a set of standardized questions. These questions involve not only their assessment of the beamline/endstation, but their experiences at the facility as a whole. Upon responding, beamline staff can review their feedback while the user remains anonymous. Negative comments often speak to facility issues rather than beamline issues, i.e. beamdumps, bad lunchroom / no canteen, bad wifi. Positive comments mention: friendly and very knowledgeable staff who give a lot of help through the whole experiment.

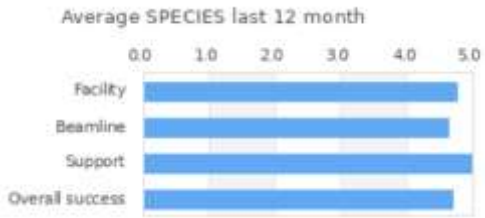


Figure 29. Feedback statistics for the past 12 months taken in March 2024.

Users are also required to submit an experimental report within three months after their experiment. The beamline staff monitor incoming experimental reports and use those to estimate the success of the experiment and publication probabilities. Experimental reports also may affect the success of future proposals: if a user (main proposer or PI) misses to send in an experimental report the score of any future proposal by that user (main proposer or PI) is reduced by 1 point.

# 4 User community and in-house research

## 4.1 User science programme

The SPECIES beamline caters to many scientific disciplines spanning from material characterization to surface science to heterogeneous catalysis to the growth of atomically thin films. The beamline publication statistics from the user science programme are plotted in Figure 30~~Figure 30~~ accompanied by their median impact factors (2021 values). The publication numbers appear to follow an increasing trend year-by-year. Further analysis has shown that users have approximately a two-year delay between experiment and publication, which clearly explains the slower uptick in publication numbers compared to the number of proposals. The number of publications associated with APXPS beamtimes clearly outmatches RIXS, but this is to be expected as it follows the same trend in the proposal numbers.

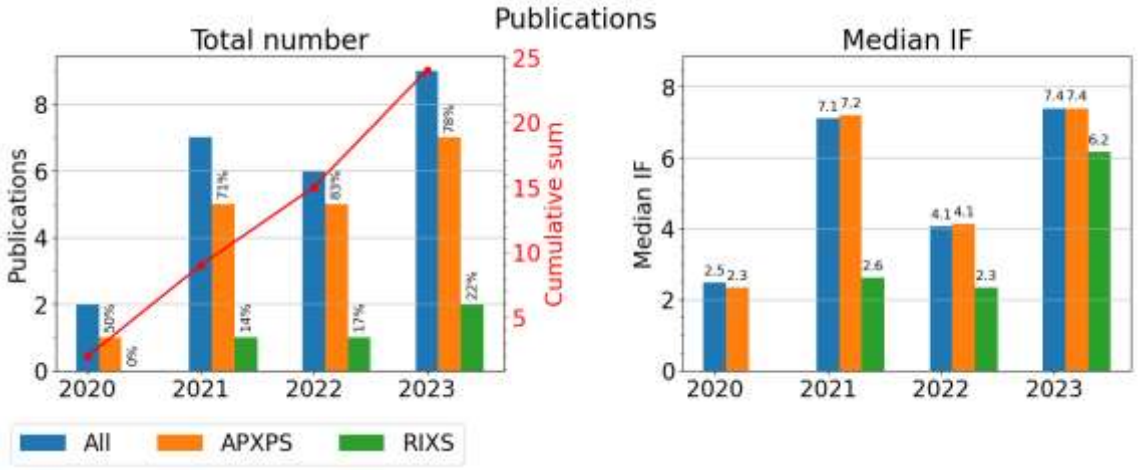


Figure 30: Left: all publications affiliated with SPECIES since 2020 and sorted by branch. Note that in 2020 and 2021, there were publications that did not originate from either branch (beamline papers). Right: the median impact factor (IF) from all publications sorted by year. Impact factor data is from 2021.

Key scientific areas were identified after assessing the scientific content within all beamline publications (Figure 31~~Figure 31~~). The low-energy RIXS endstation provides a platform for UHV material characterization of electronic correlations in valence electrons (publications: **3**). UHV material characterization is also performed at SPECIES-APXPS usually in combination with other techniques to augment a multi-modal study (**3**). However, the APXPS endstation excels at *in situ* monitoring of a material under relevant conditions for surface science (**11**), heterogeneous catalysis (**4**), atmospheric science (**1**), and ALD film growth (**5**), which can be applied to certain scientific fields, i.e. battery research (**2**) and solar cell technology (**2**), and notable materials classifications, i.e. 2D materials (**1**). Note that "UHV material characterization" is defined as a UHV measurement without gas exposure, "surface science" refers to an adsorption/desorption experiment that involves one gas interacting with a material, and "heterogeneous catalysis" details a chemical reaction taking place on a catalyst to which a mixture of gases is expected. Technical papers are also included within the science areas (orange) along with beamline development efforts (**3**) and scientific reviews (**1**).

To highlight the capabilities of the SPECIES beamline, we present in the following user science cases from most of the scientific areas outlined in Figure 31~~Figure 31~~.

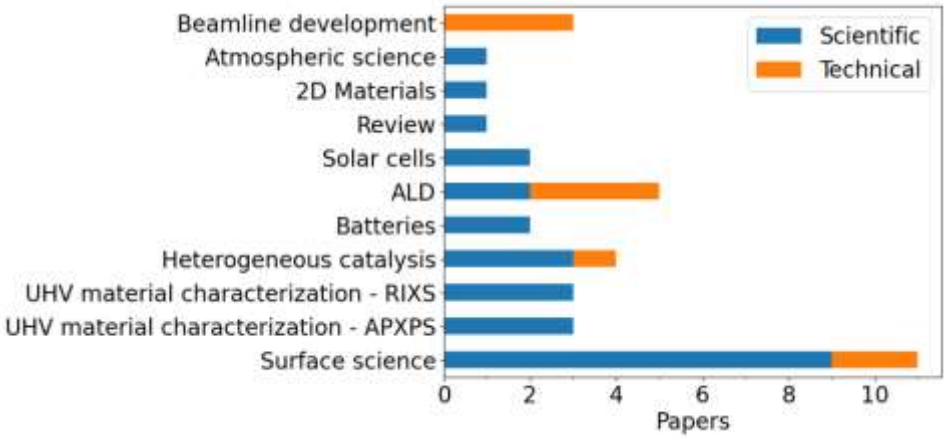


Figure 31. SPECIES publication statistics classified according to scientific disciplines and applied fields.

**UHV material characterization using RIXS:** A combination of soft X-ray RIXS and XAS provide a platform for understanding quantum phenomena in correlated and energy materials, such as superconductivity and charge and spin excitations. RIXS provides chemical- and site-selective information by mapping out the energy and momentum loss of these low-energy excitations. Prof. Yasmine Sassa's group analyzed the origin of charge density waves (CDWs) in layered $LaPt_2Si_2$ that previously demonstrated superconductivity and CDWs at different temperatures (Figure 32~~Figure 32~~)[14]. Their study showed the cause of CDWs stemmed from a lattice distortion due to the breaking of inversion of symmetry between two seemingly similar Si-Pt-Si layers.

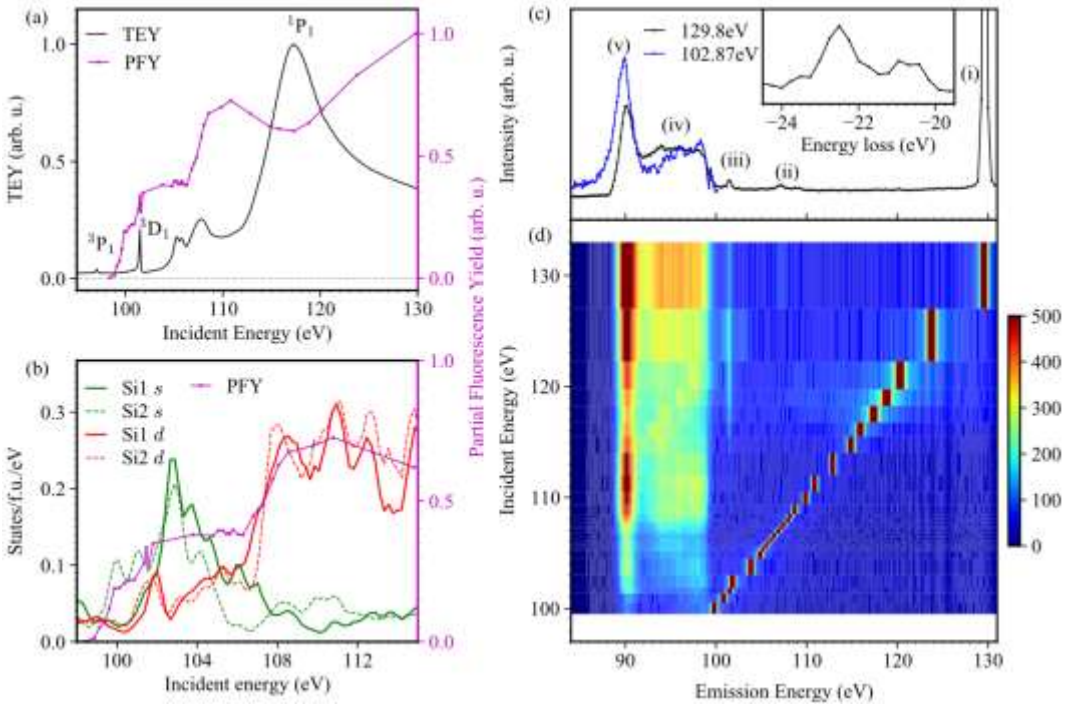


Figure 32. RIXS study of charge density wave formation in $LaPt_2Si_2$[14].

**Surface science applied to batteries:** SPECIES is particularly suitable for Li-ion battery research due to the beamline photon energy range that enables surface sensitive measurements of the Li 1s core-level as well as

[14] Mukkattukavil, D.J., *et al.*, *Journal of Physics: Condensed Matter*, 34, 324003 (2022).

depth profiling capabilities. Doc. Maria Hahlin's group probed electrolyte effects at an electrode/electrolyte interface relevant in Li-ion batteries by studying a liquid droplet of Li salt in propylene carbonate (electrolyte) on Li metal (electrode) compared to pure propylene carbonate solvent (Figure 33~~Figure 33~~)[15]. They demonstrated a concentration gradient in the Li-salt electrolyte surface compared to the bulk. To probe the buried interface, higher photon energies with reasonable flux are needed, thus this type of study would benefit from the proposed new grating at the SPECIES beamline as outlined further in section 5.2.

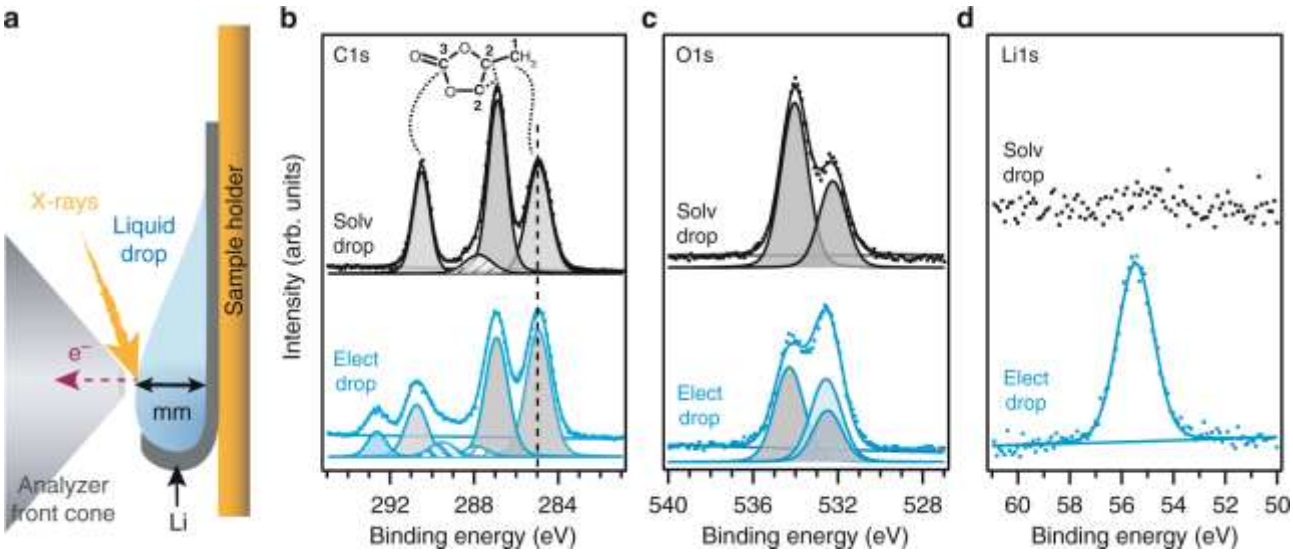


Figure 33. APXPS analysis of a liquid droplet of propylene carbonate (Solv-Drop) and Li-salt in propylene carbonate (Elect-drop) on Li metal to investigate electrolyte effects at a relevant electrolyte/electrode interface in Li-ion battery research[15].

Another related study from the same research group targeted the investigation of a promising Li electrode material embedded with Ni-rich transition metal oxide particles with a focus on understanding the electrode stability in different atmospheres mimicking that of air, i.e. $CO_2$, $O_2$, $H_2O$ mixtures[16]. Their results show irreversible degradation effects when interacting with $CO_2$ in the presence of $H_2O$, thus demonstrating the detrimental effects of a humid environment that should be considered in the practical use and handling of these materials in batteries.

**Industrial surface science:** Some industrial processes, such as metallurgical reduction, require very high temperatures for activation alongside harsh environments. Doc. Samuli Urpelainen's group collaborates with the steel industry to study the reduction of their industrial Fe ore pellets under practical conditions using APXPS[17]. Steel production relies upon the use of either blast furnaces (BFs) or electric arc furnaces (EAFs) to melt down Fe ore amongst other metals in a reducing environment, however this also leads to unwanted $CO_2$ emissions. CO is the reducing agent in BFs whereas a mixture of CO and $H_2$ originate in electric arc furnaces; $CO_2$ emissions are highest in BFs, thus supplying the need for a different methodology to reduce $CO_2$ emissions and utilize $H_2$ instead or in combination with CO. Doc. Urpelainen's group investigated this possibility by systematically tracking the evolution of Fe oxide to metallic Fe in each pellet type under elevated temperatures up to 650 °C in $H_2$ and CO environments. Noting the degree of metallization and changing gas flow rates for better diffusion properties, tweaking the gas mixture to promote reduction, and increasing temperature to instigate the final phase transformation from Wüstite to metallic iron. This experiment demonstrates the need for high temperature reaction environments which currently pushes the capabilities of the available heater. Therefore, the on-going project to replace the cell with a high

[15] Maibach, J., *et al.,* *Nature Communications*, 10, 3080 (2019).
[16] Chen, H., *et al.,* *ACS Applied Energy Materials*, 6, 22, 11458-11467 (2023).
[17] Heidari, A., *et al.,* manuscript submitted (2024).

temperature catalysis cell using laser heating will open up the possibility of probing close to industrial standards needed for these types of experiments and more.

**Heterogeneous catalysis:** Heterogeneous catalysis studies including model catalysis, industrial catalysis, and photocatalysis feature prominently in the research proposed and performed at SPECIES-APXPS using the catalysis cell. The setup features an unique experimental set-up for mixing gases due to the double cone gas inlet system attached at the front of the cell (see Figure 9~~Figure 9~~ for a flow simulation) coupled together with heating capabilities for thermal activation and a port/window to introduce an external light source for photoactivation of a catalyst. Sample complexity can be an issue especially for industrial and photo-catalysts that usually involve supported nanoparticles on powders. Due to their inherent electrically insulating nature, charge compensation can be required under synchrotron radiation; fortunately, the setup is well equipped for this purpose and can introduce gas to compensate for charging effects. Here, we present a few examples of the types of heterogeneous catalysis we do at SPECIES-APXPS.

**Industrial catalysis:** Currently, industrial methanol synthesis uses Cu/ZnO as a catalyst, however, it suffers from selectivity issues and the need to use solvents in the $CO_2$ hydrogenation reaction. Dr Abdel-Mageed's group took a different approach by adding Au into the industrial catalyst creating a bimetallic $Cu_xAu_x$ nanoalloy supported on ZnO (Figure 34~~Figure 34~~)[18]. In their multi-modal study, they show that Au acts to stabilize Cu leading to the reduction of Cu oxidation, negating the need for solvents, and reporting full conversion of reactants to methanol in an aqueous environment. Depth profiling under reduction and reaction conditions showed segregation of Cu at the surface compounded by a thin surface alloy with Zn while Au migrates to the core of the particles confirmed by other methods as well. Interestingly, under a mixture of $CO_2$, $H_2$, and $H_2O$ atmosphere, APXPS studies revealed an active intermediate at 200 °C attributed to adsorbed methoxy- or formate-type species whose signal was minimized upon heating to 250 °C alongside an increase in methanol production. The work reveals the key mechanistic finding that allows methanol formation at temperatures as low as 250 °C.

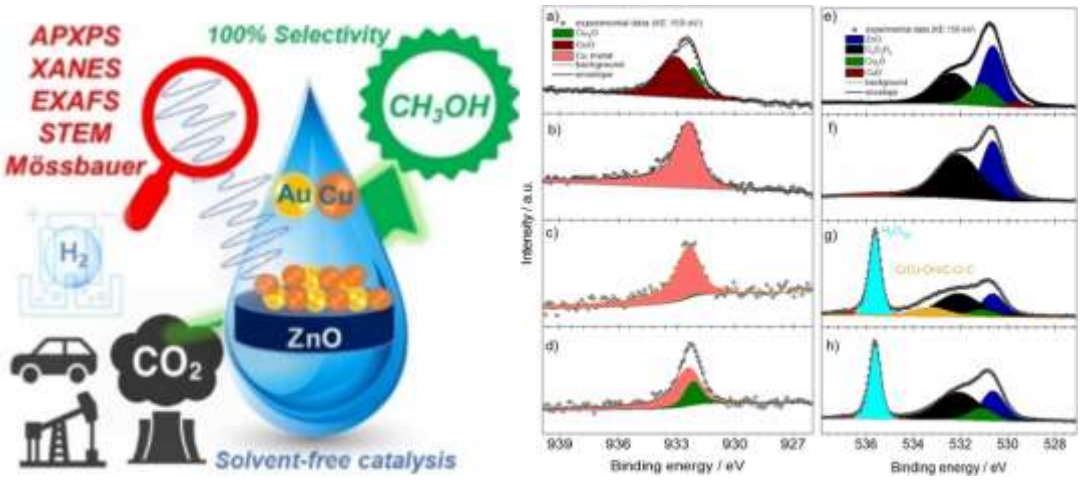


Figure 34. A multi-modal study claiming 100% selectivity towards methanol in the $CO_2$ hydrogenation reaction taking place in an aqueous environment containing an industrial catalyst composed of bimetallic $Cu_xAu_x$ nanoalloy supported on ZnO[18].

**Time-resolved in model catalysis:** Pushing at the boundaries of traditional model catalysis, Doc. Jan Knudsen's group uncovers hidden surface structure in catalytic reactions taking place on well-studied single crystals using time-resolved APXPS and reconstituting an analysis approach not commonly used in XPS but

[18] Mosrati, J., *et al.*, *Angewandte Chemie International Edition*, 62, e202311340 (2023).

proves to have impactful results[19]. Taking advantage of the small volume cell with a double cone for fast gas introduction at the front of the sample and efficient pumping, the users pulse gas from mass flow controllers or fast piezo valves to push the time-resolution to detect metastable species in catalytic reactions on millisecond timescales. This pulsing scheme and the fast detection speed of the delay line detector provides an excellent experimental platform for signal event-averaging to enhance XP spectra which can be further analyzed using a fast Fourier transform technique to detect species even within the noise level. The users' latest submitted manuscript illustrates this science on the CO oxidation of Pd(111) where an unusual active phase was observed, i.e. the CO-covered surface is the active component rather than the widely presumed chemisorbed oxygen or oxide phase[19].

**Photocatalysis applied to solar cells:** SPECIES users benefit not only from thermal means of initiating a chemical reaction as addressed above, but also from using an external light source provided at the beamline that mimics the solar spectrum and photoactivates a reaction. In this way, solar cell materials can be appropriately studied, through light activation as well as under relevant sample environments aimed at their intended outside installation, i.e. exposed to air and varying weather conditions. For example, the Fahlman research group systematically studied the stability of a promising organic-organic semiconductor interface, namely layers of PM6:Y6, when exposed to $H_2O$, $O_2$, and light at near-ambient conditions[20]. The blended organic films showed enhanced stability towards $O_2$ and $H_2O$ as compared to their independent counterparts, particularly Y6 where degradation was initially detected under ambient pressures when studied alone. Furthermore, taking advantage of high flux at low photon energies, the group assessed the interfacial chemistry in the valence band, specifically at the Fermi level. The measurements showed reversible p-doping effects of the blended films in the presence of oxygen, a finding that could impact the use of this photoactive material in a solar cell device.

**Atmospheric science:** With the advent of dense population areas and industrial complexes, aerosol output has increased, affecting the natural atmospheric cycles with sometimes detrimental consequences, i.e. air pollution, depletion of the ozone layer, etc. To assess the chemical reactivity of common aerosol particles, Prof. Prisle's research group specially deposits isolated aerosol particles onto supports to mimic free particles and studies the atmospheric chemistry of water uptake by controlling relative humidity in the AP cell. To satisfy the full range of relative humidity values (0-100%), the sample stage containing the heater is switched to one that has a cooling capabilities and an external chiller is used to cool down the sample. This avoids the need to use very high pressures to reach high relative humidities without sacrificing spectral quality and time. In the future, the addition of a Peltier element is considered as an alternative cooling source. Under these conditions, the users evaluated phase transformations upon water uptake in NaCl, sucrose, and malonic acid as featured in Figure 35~~Figure 35~~[21]. In general, surface sensitivity is crucial to these kinds of measurements especially when probing lower lying core-levels such as Cl 2p and S 2p, SPECIES beamline is the perfect platform for this energy range with high flux at low photon energy.

[19] Knudsen, J., *et al.*, in review at *Nature Catalysis* (2024).
[20] Zhang, Q, *et al.*, *Journal of Materials Chemistry C*, 11, 3112-3118 (2023).

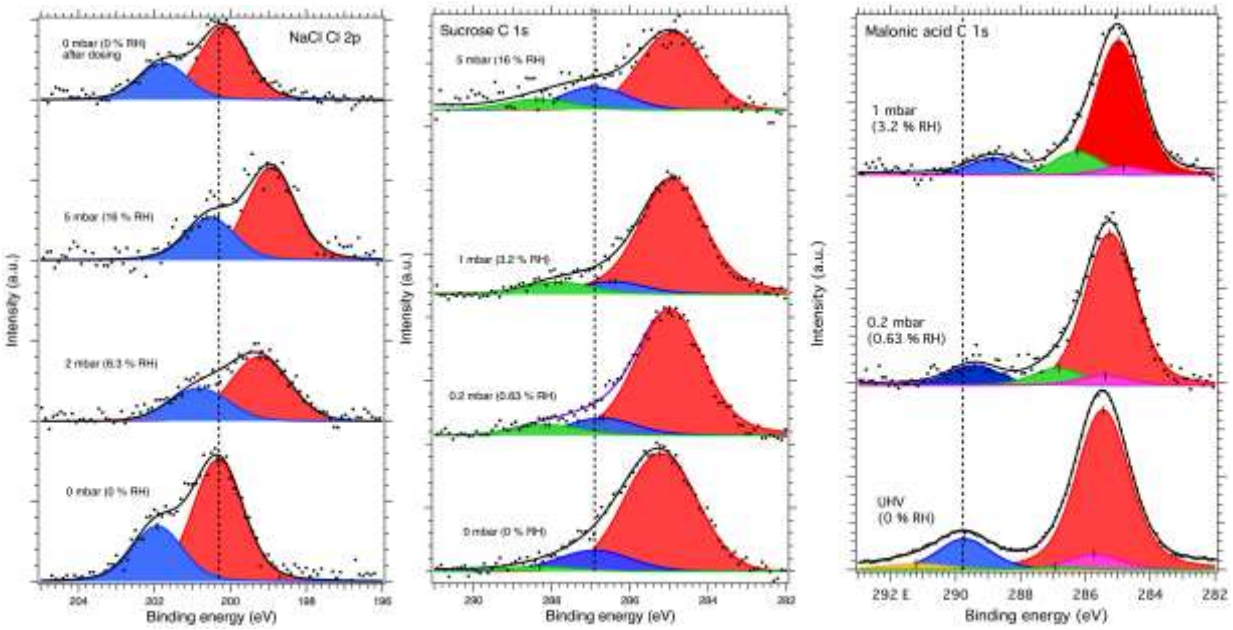


Figure 35. Investigation of the effect of water exposure in different atmospherically relevant aerosol particles including NaCl, sucrose, and malonic acid[21].

**ALD:** The working principle behind the ALD growth process so often used in making highly reproducible thin films for high performance electronic devices, i.e. field-effect transistors, relies upon precise thickness control by depositing one atomic layer at a time and covering the entire surface of the material, no more, no less. In reality, this is not always the case, particularly at the interface between different materials where a sharp interface is crucial to promote efficient charge transfer in devices. Using the dedicated ALD cell, Prof. Schnadt's and Doc. Timm's research groups investigate interfacial effects in the ALD growth of $HfO_2$ on InAs using time-resolved APXPS to determine the reaction mechanism and dynamics (Figure 36~~Figure 36~~)[22]. They discovered that the surface of InAs plays a critical role and strongly influenced the growth of the first half cycle of TDMA-Hf precursor. TDMA-Hf reacted with oxygen contaminants on the surface to produce $HfO_x$ already in the first half cycle. In the second half cycle, $H_2O$ reacted with organic surface species, i.e. cleaning the surface, and created a uniform $HfO_2$ film with some -OH terminated species. To fully saturate the surface and produce the best film quality, long exposure times were required for each half cycle. Thus, proving an excellent methodology to produce a sharp interface at this industrially relevant interface using the unique ALD cell that is only found at the SPECIES beamline.

[21] Lin, JJ, et al., *Atmospheric Chemistry and Physics*, 21, 4709-4727 (2021).
[22] D'Acunto, G., *et al.*, *Surfaces and Interfaces*, 39, 102937 (2023).

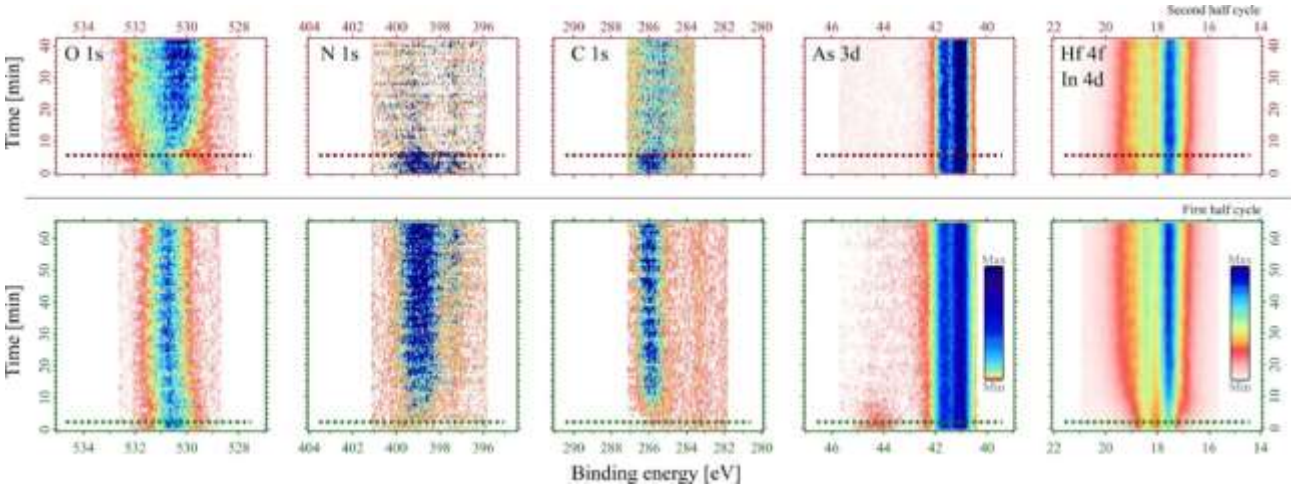


Figure 36. Time-resolved APXPS of the first and second half cycles of the ALD growth of $HfO_2$ grown on InAs using a TDMA-Hf precursor and $H_2O$, respectively[22].

## 4.2 In-house research activities

The in-house research activities at SPECIES are often aimed at new developments and testing new beamline capabilities. In some cases, pure science is done as well, but this portion has remained rather small. Here we will describe in more detail some of the ongoing in-house projects.

The amount of in-house used can be seen in the proposal statistics in Figure 22~~Figure 22~~.

Typically, in each cycle, approximately 25 % of all beamtime goes towards in-house research (IHR) activities. In the MAX IV terminology, IHR also contains all beamline commissioning beamtime. Since the nature of IHR is very experimental, it is expected that the probability of getting published results from each IHR beamtime is therefore rather smaller than in normal beamtime. As an example, the list of IHR beamtimes in 2023 include:

- Research into ethanol dehydrogenation of nitrogen-doped graphene (postdoc research, explained in more detail below in section 4.2.2).
- Investigating the electronic structure of propylene carbonate in gas phase (a short beamtime which was a continuation of research from an older IHR experiment which is expected to yield publishable results.)
- Testing the feasibility of the combination of temporal analysis of products (TAP) and APXPS. (a collaboration with University of Oslo to develop a novel setup for gas phase perturbation based experimental setup to study kinetics of catalytic reactions).
- Expanding the scope of ALD precursors and light activation (see below in section 4.2.1).
- Using beamline commissioning time to develop the PGS and obtaining first RIXS results from that spectrometer.

Since 2020, all IHR work has resulted in 4 papers. These are:

- E. Kokkonen, *et al.*, *Ambient Pressure X-Ray Photoelectron Spectroscopy Setup for Synchrotron-Based* in Situ *and* Operando *Atomic Layer Deposition Research*, Rev, Sci. Instrum. **93**, 013905 (2022).
- E. A. Redekop *et al.*, *Synchronizing Gas Injections and Time-Resolved Data Acquisition for Perturbation-Enhanced APXPS Experiments*, Review of Scientific Instruments **92**, 044101 (2021).
- E. Kokkonen *et al.*, *Upgrade of the SPECIES Beamline at the MAX IV Laboratory*, J. Synchr. Rad. **28**, 588 (2021).
- A. Klyushin, *et al.*, *Photocatalytic Setup for* in Situ *and* Operando *Ambient-Pressure X-Ray Photoelectron Spectroscopy at MAX IV Laboratory*, J. Synchr. Rad. **30**, 613 (2023).

There are some papers where work done on IHR beamtimes gets mixed up with proper PAC proposals, and it is therefore not trivial to identify all work accurately. In addition, some published work gains valuable insight and learning experiences from an IHR beamtime even though no published results come out of it.

### 4.2.1 Expanding ALD portfolio with new precursors and light activation.

The deposition of oxides, for example in the case of gate oxides or high-K dielectric films requires the use of a precursor capable of supplying reactive oxygen on the surface of the film. Typical precursors are $O_2$, $H_2O$, $H_2O_2$, and $O_3$. Especially in the ALD of high-K dielectric films, ozone has distinct advantages over the alternative oxidizing agents: high electrochemical potential resulting in fast reaction rates at low temperatures while being highly volatile, thus shortening purge times between cycles. Another crucial difference is the pumping speed of $O_3$ is much faster compared to $H_2O$ or similar. For these reasons, we thought it pertinent to explore the possibility of using ozone in the ALD cell for potential user operation in the future.

Practically speaking, the ozone was produced in an ozone generator fed with pure oxygen. The flow was adjusted to produce as high a concentration of ozone as possible, and a small portion of the flow was directed to one of the inlet lines of the ALD cell via an adjustable vacuum leak-valve. The leak-valve was used to adjust the pressure inside the cell. However, in this experiment, the valve was manually operated making the ozone "pulses" rather long and undefined. This scheme also allows us to leak pure $O_2$ into the cell simply by keeping the ozone generator turned off. The gas that was not leaked into the cell was directed into the ventilation system after passing through an ozone scrubber. We estimated the ozone concentration to have been in the range of 5-10 %.

The deposition of $HfO_x$ on silicon substrates was chosen as the target study. Many studies have been done on these systems in the past[23], but they have all focused on using $H_2O$ as the co-reactant. The effect of temperature dependence in the deposition was also explored.

Data was collected both before and after two full cycles, but also during the deposition itself. Figure 37~~Figure 37~~ shows the N 1s spectra recorded before and after the deposition at various stages and different temperatures.

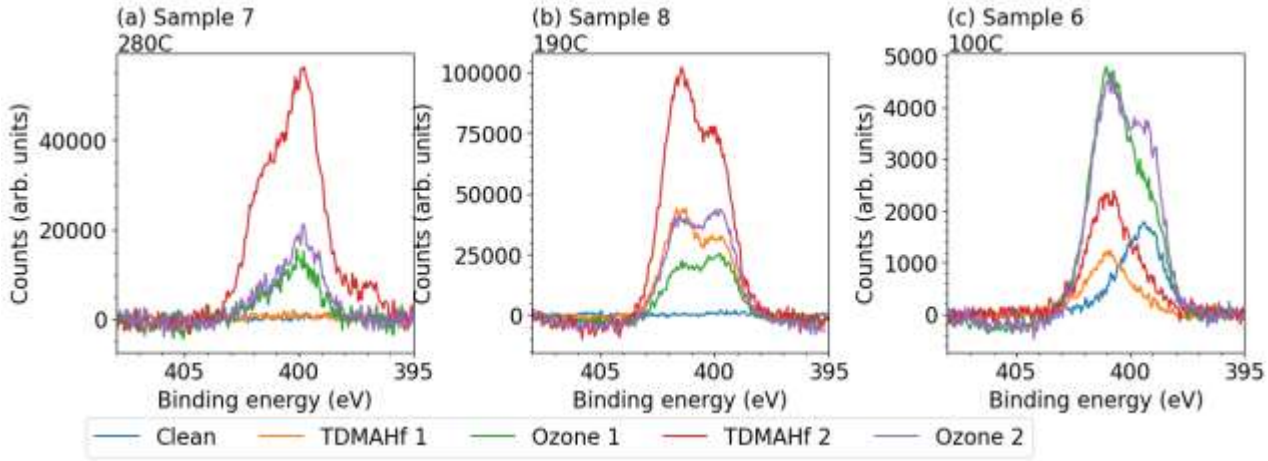


Figure 37. The N 1s spectra collected before and after half-cycles during Hf deposition.

[23] R. Jones, *et al.*, *Journal of Vacuum Science & Technology A*, 42, 022404 (2024).

In addition to ozone, a pulsed UV source has also been commissioned to use in conjunction with the ALD cell[24]. This work has been done in collaboration with Associate Prof. Ville Miikkulainen from Aalto University in an effort to study the photo-assisted deposition of high-k oxides and metals. Photo-ALD offers a facile route to the patterning of substrates avoiding harsh chemical treatments by utilizing the underlying substrate photoactivity[25].The initial commissioning focused on successfully depositing $HfO_2$ and Cu metal via photo-assisted ALD. Initial results show the oxidation of Hf-butoxide to $HfO_2$ over time (Figure 38~~Figure 38~~), for proof-of-concept, UV exposure was carried out without measurement.

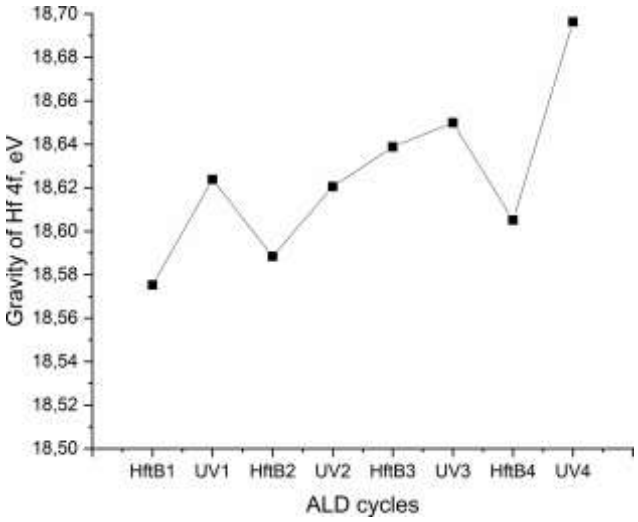


Figure 38: The first moment of the fitted Hf 4f over 4 cycles (8 half cycles) of a hafnium tert-butoxide (HftB) and UV pulses. The shift to higher binding energy is indicative of $HfO_2$ formation.

Further investigation into the exact mechanisms involved in photo-ALD is now planned, with the aim of also improving the automation of the photo-ALD half-cycles by further enhancing the control automation.

### 4.2.2 Tracking the catalytic mechanism in a functionalized 2D material

Using the highly optimized AP catalysis cell at SPECIES-APXPS, the potential of nitrogen-doped graphene as a novel catalyst in heterogeneous catalysis was studied, specifically the ethanol dehydrogenation reaction. Heteroatom doping of graphene creates reactive sites at and around the dopant sites, thus promoting different levels of reactivity and selectivity based upon the dopant site type and doping level in an otherwise inactive graphene sheet. The experiment uses a $N_2$ plasma to insert nitrogen atoms controllably and reliably into the graphene lattice either substitutionally (graphitic N), additionally with carbon defects (pyridinic N), or through ring changes from a 6-membered ring to a 5-membered ring (pyrrolic N). The evolution of reaction intermediates was systematically tracked in the ethanol dehydrogenation reaction at elevated temperatures steps using APXPS and APXAS.

Ethanol dehydrogenation ideally produces value-added chemicals, i.e. acetaldehyde, however this reaction suffers from selectivity issues and is prone to undergo side reactions or result in decomposed products. Ethanol interaction was investigated with several nitrogen-doped graphene films which produced distinctly different reaction mechanisms due to their initial nitrogen dopant concentration and dopant types (Figure 39~~Figure 39~~)[26]. A moderate dopant concentration (4% N:C) with a high percentage of graphitic N converts to pyrrolic N under ethanol vapor and relies heavily upon nitric oxide intermediates to catalyze the reaction. In contrast, heavily doped films (7% N:C) with primarily pyridinic N sites results in a basic backbone which

[24] A. Klyushin, *et al.*, J. Synchrotron Rad. **30**, 613 (2023).
[25] V. Miikkulainen, *et al.*, Adv. Materials. Inter. **8**, 2100014 (2021).
[26] Eads, C.N., *et al.,* in preparation (2024).

promotes interaction with carbon atoms next to nitrogen sites. These results elucidate selectivity pathways and reveal the need for control of nitrogen dopants in the defect engineering of nitrogen-doped graphene as a next generation catalyst.

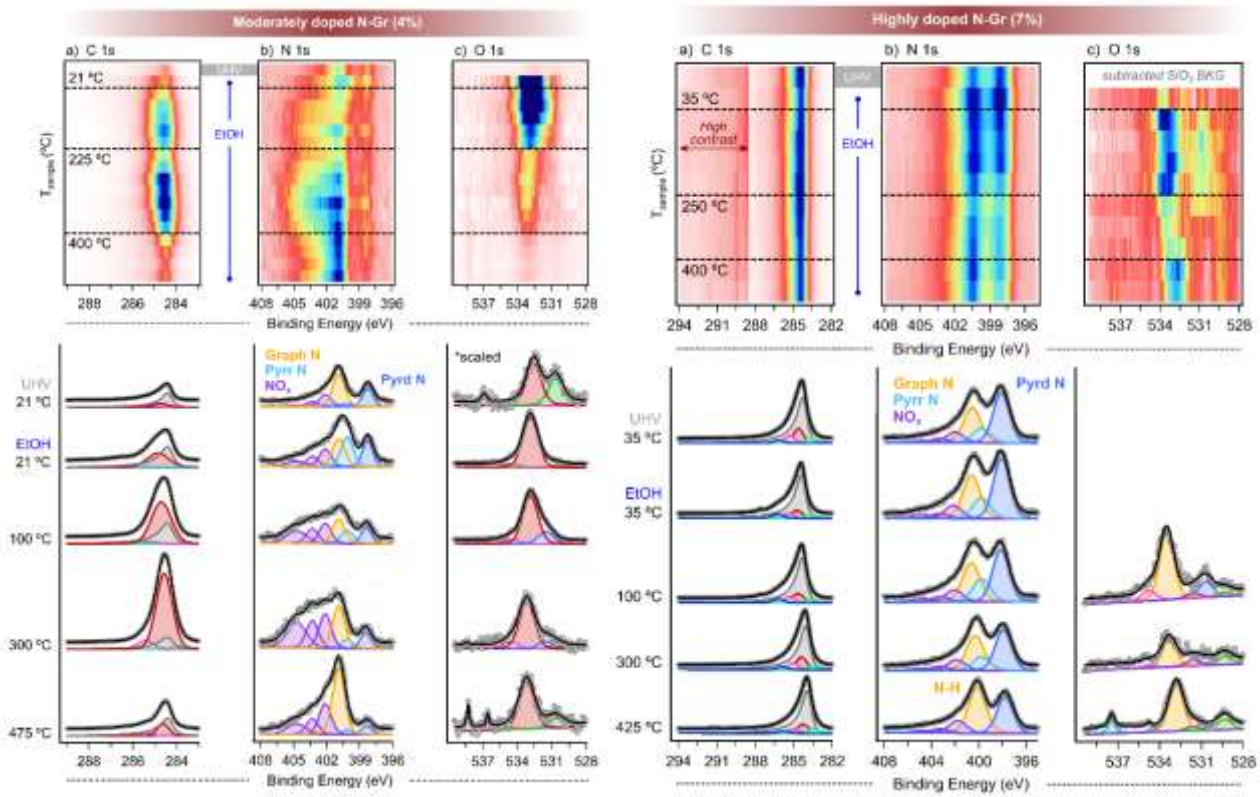


Figure 39. APXPS study of the ethanol dehydrogenation reaction of N-Gr with varying N-doping levels (left: 4% N:C, right: 7% N:C) leading to vastly different reaction mechanisms[26].

### 4.2.3 Development of photocatalysis

Processes driven by solar radiation play a crucial role in life on Earth. Presently, one of the most significant challenges confronting modern human civilization is the shift from fossil fuels to clean and renewable energy sources. By irradiating the photocatalyst and causing the generation of electrons and holes, natural photo-assisted solar reactions can convert solar energy into usable chemical energy. However, there is a lack of APXPS studies that pair synchrotron light with external light sources. Therefore, the AP cells were developed to transmit solar/UV light from an external light source mounted outside the analysis chamber to illuminate the sample inside the cell (Figure 6~~Figure 6~~).

Hydrogen production through water splitting is one example of a scientific application where sunlight is used to trigger a photocatalytic reaction at a photoactive surface. As photocatalysts, pristine Ni@NiO/$NiCO_3$ core-shell nanostructures were examined while monitoring electronic structure evolution using APXPS under solar simulator irradiance[27]. During illumination, the metallic Ni peak was observed to vanish, and a new peak that we identified as NiOOH developed (Figure 40~~Figure 40~~). Conversely, there were no changes observed in the Ni 2p peaks originating from NiO and/or $NiCO_3$.

[27] A. Klyushin, *et al.*, J. Synchrotron Rad. **30**, 613 (2023).

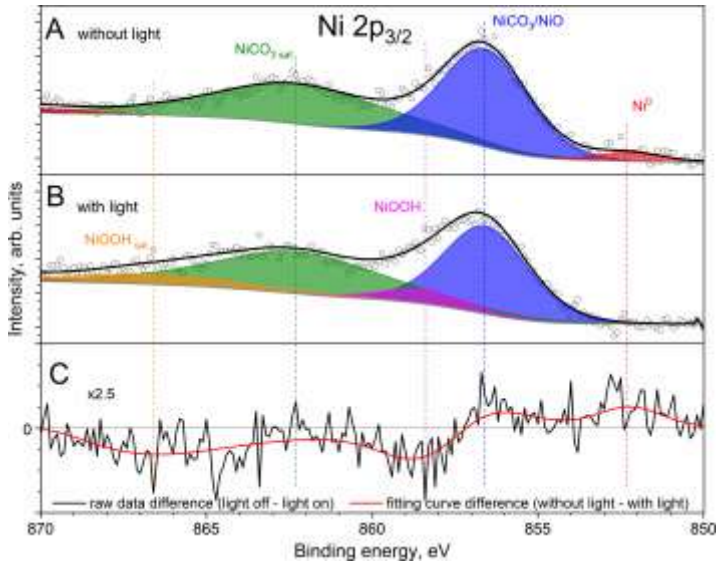


Figure 40. Ni $2p_{3/2}$ spectrum of in situ APXPS studies of the hydrogen evolution reaction on Ni@NiO/$NiCO_3$ at room temperature under 1 mbar $H_2O$.

### 4.2.4 RIXS commissioning and detector development

Until now, the in-house activities at the RIXS branch have been focused on the various development projects and general endstation commissioning. Bringing the PGS instrument into user operation will mark the end of this phase.

## 4.3 Benchmarking

The beamline is benchmarked against similar beamlines at other synchrotrons. While all beamlines often have their own user communities that place demands on sample environments and such, they are often similar enough that they can be compared in order to analyze the performance and output of the beamline.

For benchmarking purposes, the RIXS endstation at SPECIES is compared to SEXTANTS beamline at SOLEIL synchrotron, which has a similar flux, spot size, and resolution (Table 3~~Table 3~~). The beamline is also the only one with a comparable energy range to SPECIES that's currently in user operation. From the comparison, SPECIES-RIXS offers high photon flux at low energies with also quite high resolution. Challenges still remain, which is evident in the number of publications originating from the compared beamlines.

Table 3. SPECIES-RIXS benchmarking.

| RIXS branch | SPECIES* (MAXIV) | SEXTANTS* (SOLEIL) |
|---|---|---|
| Operation started | 2022 | 2010 |
| Publications after 4 years | 4** | 32 |
| Energy range [eV] | 30-1500 | 50-1700 |
| Flux | $1x10^{13}$ (@100 eV) | $1x10^{14}$ (@ 100 eV) |
| Resolving power | 10000 @ 400 eV | 10000 up to 1200 eV |
| Spot size | 5 x 25 | 80 x 2 |

*Branched beamline
**Only RIXS related publications

The APXPS branch can be compared to numerous beamlines at many different synchrotrons around the world. Here, we have chosen beamlines with similar photon energy ranges (Table 4~~Table 4~~). Compared to most other beamlines, SPECIES offers possibilities with high flux at low energies providing capabilities for AP-UPS, which has limited accessible elsewhere. Within the compared beamlines, the sample environment

capabilities are also very similar. Of course, some unique capabilities likely exist at every beamline, such as the ALD cell at SPECIES. The number of publications after four years of operation appears to be on a similar level to the compared beamlines with the exception of VerSoX. VerSoX beamline is an interesting comparison, as the high productivity of the NEXAFS endstation appears to drive a lot of publication potential.

Table 4. SPECIES-APXPS benchmarking.

| APXPS branch | SPECIES* (MAXIV) | TEMPO* (SOLEIL) | Circe* (ALBA) | 11.0.2* (ALS) | VerSoX* (Diamond) | ISISS (BESSY) |
|---|---|---|---|---|---|---|
| Operation started | 2019 | 2014 | 2013 | 2005 | 2019 | 2007 |
| Publications after 4 years | 19** | 5 | 12 | 11 | 38 | 18 |
| Energy range [eV] | 30 - 1500 | 40 - 1500 | 100 – 2000 | 75 - 1400 | 260 - 2600 | 80 - 2000 |
| Flux (energy, resolution) | $1x10^{13}$ (@400 eV, R=5000) | $3x10^{12}$ (@800 eV, R=5000) | $1x10^{13}$ | $1x10^{13}$ (@400 eV) | $1x10^{11}$ | $6x10^{10}$ (@400 eV, R>15000) |
| APXPS pressure / temperature | 20 mbar / 5 - 600 °C | | 25 mbar / -23 - 700 °C | | 30 mbar / RT - 500 °C | 20 mbar / RT - 700 °C |

*Branched beamline
**Only APXPS related publications

# 5 Developments: ongoing, planned, and possible

## 5.1 Missing design capabilities

**APXPS Gas system**

The transfer package from the MAX-lab to the MAX IV Laboratory included the new gas system. However, the gas system's implementation is still not finished at the time of writing this report (for the reasons, see below). Instead, two small ventilated cabinets were put in as a temporary solution. As a result, the current temporary gas system's inflexibility limits the complexity of feasible experiments. In addition to the number of hazardous gases, their volume is restricted to 1 liter, which occasionally requires changing the bottles during beamtime. Furthermore, the gas bottles are required to be attached at the beginning of the experiment and to be removed immediately after beamtime, which raises the possibility of installation-related human error because of very frequent gas bottle installations.

The new gas system will reduce the need for bottle exchanges during experiments by enabling the use of larger and higher purity gas bottles. Additionally, safety PLC enables the logging of equipment malfunctions and the monitoring of gas line status. Experiments become potentially more complex and flexible with the rise of permanently installed gases.

During the first few years, after transfer to the MAX IV site, work on the new gas system was not prioritized and due to the lack of resources caused several delays. When work could have been scheduled to start the full installation, the safety aspect of the system, designed and fully operation in the old facility, became a serious obstacle causing increased delays. It was decided that the gas system required the installation of a completely new safety system on top of the already existing equipment. Similar systems (as described earlier in section 2.5.1) were also in demand at other beamlines, which were prioritized above SPECIES in the installation. The build-up of the new safety system has been an enormous task lab-wide, requiring several hundreds of personnel hours to develop. This has understandably further delayed the implementation of the

full gas system at SPECIES. At the time of writing this document, most of the work on the gas system (and safety system) has been nearly completed with some work still being required in the software implementation and thorough testing of all the new infrastructure. The “gas projects” at MAX IV compose multi-million SEK investments that have been running for several years. The beamline staff have also contributed a high workload to the project, especially in the design phase of the safety system.

**APXPS Sulfur cell**

Sulfur chemistry and sulfur-based processes are seldom studied using APXPS at synchrotron facilities. However, such experiments are highly desirable for various fields ranging from bio-oil processing, selective heavy-metal adsorption, and catalysis. Especially processes such as hydrodesulphurization and hydrodeoxygenation that could be further investigated using appropriate APXPS instrumentation. The issue has largely been a technical one related to the lack of dedicated setups.

For this reason, a project has been on-going for some time to build a dedicated AP cell for use with sulfur-containing gases, such as $H_2S$, and sulfur-containing liquids like dimethyl sulphide and dimethyl disulphide. Realistic concerns with using most sulfur-containing gases or vapors at high pressures are their high potential for creating cross-contamination issues and corroding the instrumentation. Sulfur-containing gases commonly remain in chambers for a rather long time even after extended bake-outs. To alleviate these problems slightly, a dedicated setup could be used which can be swapped out relatively quickly to resume operations with a non-contaminated AP cell. Such cell swapping is commonplace at SPECIES with the ALD cell and could be equally easy with a dedicated cell for sulfur chemistry. However, the analyzer remains the same.

The project has faced several serious delays. One of the biggest delays was the missing gas system. Since $H_2S$ especially places heavy demands on the safety of the gas system and requires extra safety systems, cell development stopped until the entire gas system and its associated safety system was fully functional. The gas system is expected to be fully functional by the end of 2024, and therefore the sulfur cell could be usable around that time as well.

The mechanical design of the cell faces some additional technical challenges. Details such as material compatibility with the very corrosive environment have not yet been fully resolved. An additional risk is the cross-contamination with all other science at the APXPS endstation. While the cell itself would be a dedicated setup, there are still a large number of components that would be shared with all other experiments. This includes some portions of the gas outlet system but also the entire spectrometer. The pre-lens chamber especially is often at high pressure during experiments, and it is currently unclear how efficiently it can be cleaned by simply baking out the chamber between sulfur and non-sulfur experiments. A concern is that the endstation will become permanently contaminated by sulfur once sulfur experiments begin. This would prevent experiments that are especially susceptible to contaminants such as model catalyst studies using single-crystal surfaces. These concerns are currently unresolved.

## 5.2 Short-term and middle-term developments

**High-temperature APXPS cell project.**

This project aims to replace the existing “standard” cell at the APXPS endstation with a new heating system. In 2023, funding was obtained from the Crafoord foundation and SPECS was chosen as the supplier. The new cell contains several important improvements. The heating system utilizes an infrared laser that is directed towards the back of the sample plate (Figure 41~~Figure 41~~). This should enable fast and reliable heating which reaches high temperatures (up to 1000 °C). Laser heating avoids the need to place the heating element inside the cell, thus negating all the negative effects of the heater seeing the reaction environment and influencing experimental results, particularly in gas phase product formation. Crucially, the cell will be able to carry out all the existing user science programmes with minimal disruption to user operation. The aim is to switch to the new cell as seamlessly as possible, however, there will be changes to the rest of the endstation, especially in terms of added laser safety measures.

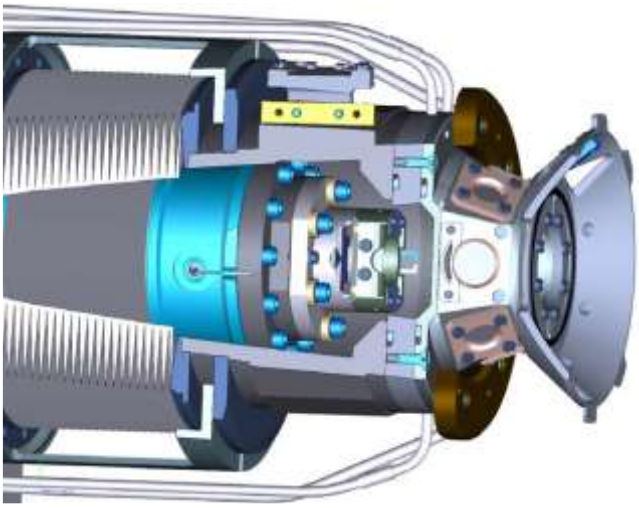

Figure 41: Schematic view of the high-temperature cell from SPECS. Sample is shown in the middle of the cut-out. The right side of the cell shows the various windows for light and sample camera as well as the docking connection to the analyzer.

The current timeline marks the delivery of the cell to MAX IV at the end of 2024. After a short commissioning and testing period, we will dedicate in-house time for expert users/collaborators. One of the scientific projects is the investigation of hydrogen reduction of iron at high temperatures – a field which promises high interest in industrial connections, especially in the green steel sector.

At the time of writing this report, the project is waiting for SPECS to provide the final design of the new cell for approval from the beamline staff.

**Low-temperature option for high-temperature APXPS cell.**

With the change of the standard cell to the high-temperature cell from SPECS, a possibility for a low-temperature cell was also postulated. An off-the-shelf product from SPECS could be purchased, allowing quick changes of the heater setup to enable cooling samples to low temperatures (down to -50 °C). This would allow to perform experiments that require access to high relative humidities or investigations where vapors need to be condensed on surfaces. For instance, one returning user group studying aerosol particles at high relative humidity would largely benefit from this cell. The project is unfunded, but we are aiming for funding acquisition in 2025. Therefore, currently the project is at the idea stage and is not actively being pursued at this time.

**Ambient pressure X-ray absorption capabilities.**

In 2023, a collaboration between the group of Piero Torrelli (at Elettra Synchrotron and CNR-IOM) to bring the established AP-XAS cell from Elettra to MAX IV for the duration of the Elettra shutdown (Figure 42~~Figure 42~~). The collaboration aims to establish knowledge sharing between the facilities and continues to offer the setup for user access during the time Elettra synchrotron is not available for users. A contract between the facilities governs the mutual relationship and ensures that during the time the AP-XAS setup is placed at the SPECIES beamline, MAX IV will offer some portion of the available beamtime to this setup through normal proposal calls.

The AP-XAS cell will be placed within the RIXS endstation at SPECIES. The endstation is already quite suitable for this as it contains a port directly facing the beam, allowing the ease of installation with only minor modifications foreseen.

The cell consists of a small, enclosed sample environment that can be pressured to atmospheric pressures. The X-rays enter the cell through an ultrathin $Si_3N_4$ window which can maintain UHV conditions in the outer

chamber. XAS can be performed in total electron yield (TEY) mode by measuring the drain current of the sample.[28]

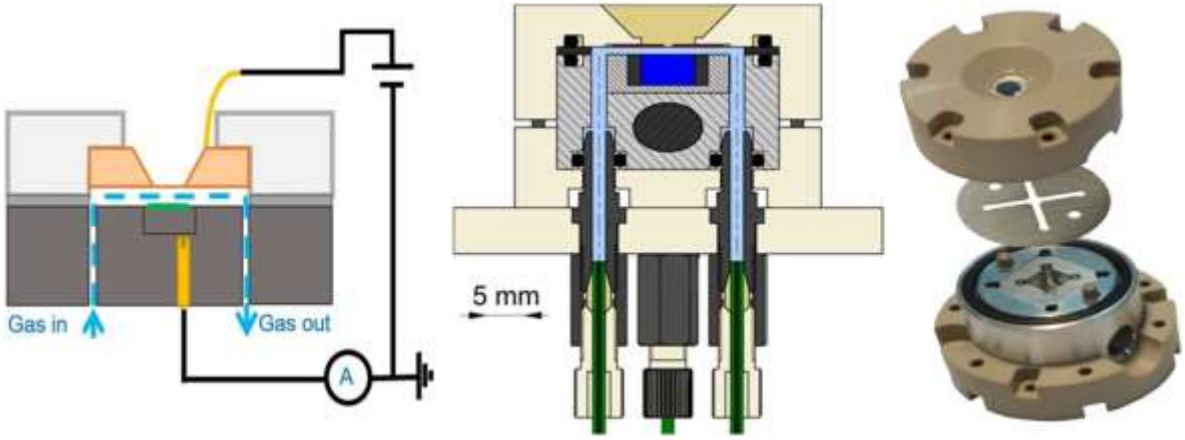


Figure 42: (Left) Electrical scheme for measuring drain current XAS with the cell. (Right): Design of the reaction cell. The cell consists of PEEK (replaced with stainless steel in higher temperature versions), Viton, aluminum, stainless steel. The sample is shown in blue color. Figure taken from ref 28.

The collaboration is expected to last until the cell is returned to Elettra (in late 2026) when the facility restarts operation. During this time, the APXPS team actively follows the progress and starts planning for AP-XAS developments of their own that could be realized at the SPECIES, HIPPIE, and Veritas beamlines.

The collaboration is currently funded completely through the operations budgets at MAX IV and at CNR-IOM. However, funding applications have been sent (for example to VR), which would further facilitate exchange of personnel at respective facilities, organization of workshops, and some small technical developments as well. The project is currently on-going with modifications to SPECIES that are needed to facilitate the Elettra cells. During summer 2024, the Elettra team will have one week of beamtime for an initial test of the AP-XAS cell at SPECIES. This test beamtime is intended to provide valuable technical feedback to modify SPECIES for the longer-term installation of the Elettra cell. The installation is expected to occur in early 2025 when in-house beamtime is dedicated to commissioning the cells for regular user operation. The cells are expected to be part of the general proposal call in spring 2025.

**Continuous energy scanning**

Continuous energy scanning is a method whereby one can seamlessly change the photon energy over the desired range with configurable speed. It is often called fly scanning or energy scanning in other places. With a soft X-ray beamline like SPECIES where the undulator harmonics are quite narrow, in practice it also means synchronizing the movement of the undulator gap and the monochromator grating and mirror axes together, so that the top of the harmonic stays within the scanned energy range for optimum flux. Therefore, sophisticated orchestration between various motors is needed. This is often realized by pre-calculating specific trajectories for the monochromator angles and the undulator gap movements. Continuous scanning is expected to greatly improve the results gained from NEXAFS measurements, by making them faster while also decreasing any noise inherent in the step scanning caused by jumping flux.

At MAX IV, there is a common project to realize continuous scanning at most of the soft X-ray beamlines. SPECIES is part of this project, and it is expected that during 2024 it will also be fully implemented into the normal repertoire of supported experiments. At the time of writing this document, the project has been implemented at a couple of beamlines (FlexPES, FinEstBeAMS, BioMAX), which should not only benefit but

[28] C. Castán-Guerrero, *et al.*, Rev. Sci. Instrum. **89**, 054101 (2018).

accelerate the implementation at SPECIES. The project requires some hardware investment (mainly a hardware controller for synchronizing the movement of the various motors) that has already been delivered. Most of the expected work is software related and therefore requires personnel hours from MAX IV software resources.

**Gas chromatograph**

For the majority of the APXPS experiments, the detection of gas phase reaction products is the key. Currently, traditional quadrupole or time-of-flight based mass spectrometers are used to monitor by-products of catalytic reactions. However, the detection limit and working principles behind these mass spectrometers are insufficient to monitor the products of some reactions. The gas chromatograph would enable experiments with a much greater detection limit, down to 1 ppm, while also allowing to separate products with similar masses and prevent gas fragmentation inside the spectrometer. Increasing the detection limit of products is a breakthrough for several research areas, such as (photo-)catalysis, model catalysis, and atmospheric physics. Therefore, the proposed equipment would significantly increase the beamline capabilities, enabling a greater variety of experiments and attracting new users from industry and academia to MAX IV. Additionally, the equipment can be utilized for operando experiments at other beamlines, including HIPPIE (APXPS), CoSAXS (scattering), DanMAX (diffraction) and Balder (XAS). A project funding application has been submitted to Crafoord Foundation; a decision is expected in summer 2024.

**New grating**

As shown in Figure 3~~Figure 3~~, the flux at high energies is lower than anticipated. One of the on-going projects is to investigate different ways of increasing the flux in this region. As the undulator power spectrum is mostly fixed and cannot be changed, the only major changes of impact are within the optical scheme. Therefore, perhaps the most obvious thing to consider is a different grating or refurbishing the optics. The gold coated grating is the oldest optical element in the beamline and will have decidedly worsened roughness, which impacts the efficiency of the grating across all energy ranges, but specifically worsens the higher energy efficiency. Currently, the project members are investigating specifications for a new grating and considering aspects such as proper line density, blaze angles, and coating materials to find a suitable compromise of flux vs. resolution. It is expected that resolution will have to be sacrificed somewhat in order to increase flux. However, since the resolution is already on the order of 400-500 meV at 1000 eV and above, we do not expect the new grating to significantly worsen this. Any increase in flux at higher energies would be beneficial to all users at SPECIES. The XPS community would likely find it valuable as virtually all XPS users use energies at 500 eV or above during their experiments. Figure 43~~Figure 43~~ shows the preliminary grating efficiency calculations for a potential lower line density grating with a range of blaze angles in comparison to the existing 1221 l/mm grating.

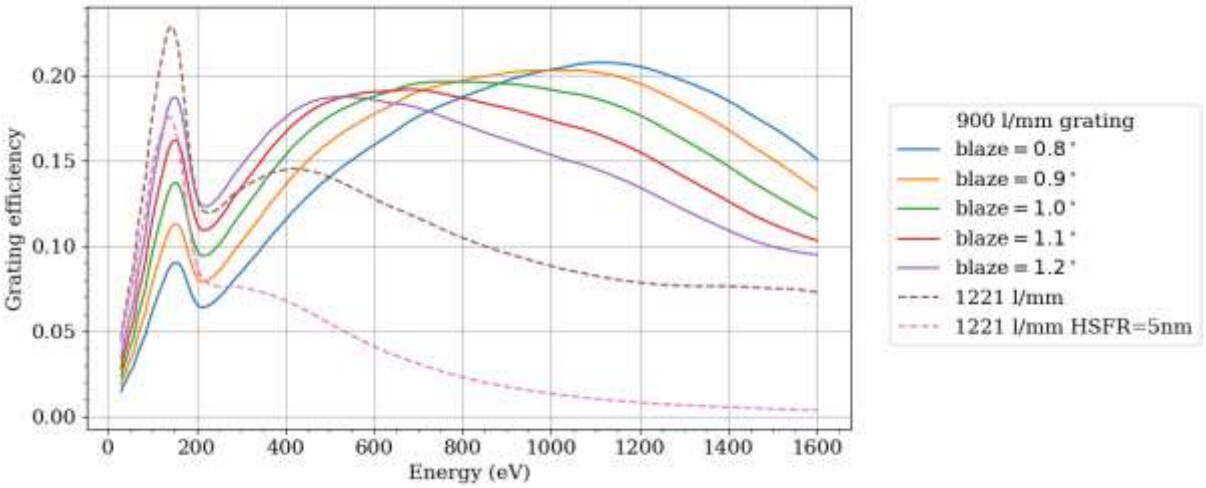


Figure 43: Calculated first order grating efficiency for a possible 900 l/mm Au coated grating with a range of blaze angles in comparison to the existing grating (dashed lines) both without surface degradation and with a roughened surface. All calculations are done with $C_{ff}$ value of 2.25. The existing 1221 l/mm grating is also compared with a nominal condition and with 5 nm high spatial frequency roughness (HSFR).

Another direction being investigated is the possibility of a grating that would be more suitable for low energies. Since RIXS is a very photon-hungry technique, any extra flux would be very valuable. Therefore, any flux increase at low energies would be appreciated by the RIXS users. Since the resolution is also very good at low energies, there could be potential for increasing flux without major detrimental effects to the resolving power.

The current stage of the project is mostly realized by the optics team at the MAX IV beamline office. The optics team are carrying out various simulations (ray tracing, etc.) to find out the optimum parameters for the two possible gratings. The project is funded completely by MAX IV (cost for ruling a single grating is estimated to be about 50 k€). We expect the delivery time of the new grating to be at least 1.5 years from the time of purchase. Since it is unfeasible to expect MAX IV to deliver two new gratings to one beamline, a decision is first needed on the necessity of one grating above the other. Therefore, the opinion of the review panel is very much appreciated. Once the grating is delivered, it would be installed during a suitable shutdown period and commissioned afterwards. Should the measured values match the desired parameters, we expect to be able to offer the new grating to users soon afterwards. However, due to the long delivery time, the new grating most likely will not be available to users before 2026.

**User friendliness by automation (APXPS)**

In order to increase beamtime effectiveness, it is desirable to automate various beamline and endstation functions as much as possible. This allows users to focus more on the scientific work and not spend too much time learning various intricacies of the beamline and endstation systems. To do this, the beamline staff spend a lot of effort on creating user friendly interfaces and tools that are intuitive for a first-time user to understand and use effectively.

Some examples of automated functions at the endstations include:

- Automated vacuum system management that operates vacuum valves in the correct order to achieve specific tasks. This means users do not need to necessarily know exactly how a task is done, as long as the end result is what they require.
- Automating repetitive tasks such as sample alignment (see Figure 44~~Figure 44~~).
- Providing complex orchestration of various parameters such as sample temperature and gas flow and pressure control. For example, if a user requires a specific temperature ramp at known gas flow conditions, this should be easily available to them in an intuitive manner.

In addition, the beamline provides some basic data analysis tools. The aim of these tools is to provide the users with a quick way of doing on-the-fly analysis to understand where the experiment is going and what the next measurement steps should be. We believe easy access to this information is paramount for effectively organizing and adapting the measurement plan. This is mostly provided in Python environments with Jupyter notebooks, but Igor Pro (with some macros) and CasaXPS are also available.

Additionally, several systems have been set up to automatically capture metadata during experiments and link it to individual measurements (spectra). The metadata includes information such as sample temperatures, various pressures, beam flux information, and others. This system allows users to be confident that they are not missing out on any important changes that could happen in the experiment that they are unaware of, since the data can be later accessed to explain, for example, unexpected spectral features.

The control system software improvements and automation tasks are projects that are nearly always running. They consist of new tasks that are added when older ones are completed. Most of the work is carried out by dedicated software personnel at MAX IV and within teams using so-called “operational resources” which are working hours dedicated to improving beamline baseline functionality and fixing common problems. However, much of this work is conducted by the beamline staff.

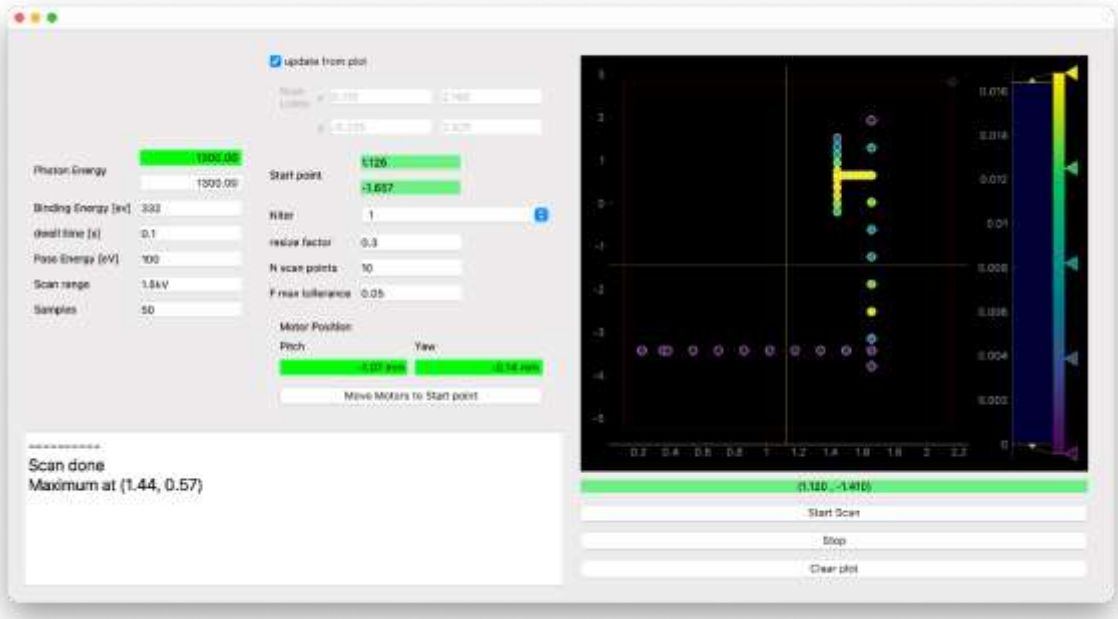


Figure 44: Example interface developed for automating the optimization process of aligning the sample to the beam during APXPS measurements.

**Upgrade of the APXPS data acquisition systems for better time-resolved experiments and obtain new detector**

The APXPS endstation currently houses a delay line detector with associated electronics (TDC) from SPECS. The current scheme allows 3D data acquisition with high spatial and time-resolved (x, y, t) resolution while also enabling the use of external signals to trigger acquisition in order to synchronize detections to any appropriate external signals. As mentioned earlier (in section 2.3.3), the measurements with the ultimate time-resolution are only possible up to a time span of 20 µs. In certain scenarios it would be interesting to push this time span even higher in order to capture more data and therefore allow for better statistics. Such a development would require changing TDC electronics. Such measurements are already possible at the HIPPIE beamline on the B-branch SPECS spectrometer.

This project is currently not pursued with very high priority due to the low demand for very high time-resolution measurements at SPECIES. However, it would likely extend the measurement capabilities quite a bit with relatively small investments.

Within the same project, the detector itself could be replaced. Currently, there is strong inhomogeneity in the detector MCP sensitivity in the energy dispersive direction. This is most likely due to very high-count rates that have damaged the MCPs over the years. This issue is rather distracting for experiments that measure a lot of low signal data using snapshot mode. To combat this, users currently have to measure extensive normalization data in order to remove the effect from the data.

The project currently lacks funding and therefore does not have a timeline. If the detector sensitivity continues to deteriorate, this project would have higher priority.

## 5.3 Major development possibilities

**Spectrometer integration project (APXPS)**

A facility wide project among all the XPS beamlines has been on-going for a couple of years. The aim of the project is to provide a unified interface for users to operate any XPS instrument independent of the manufacturer. This should benefit user experience across all beamlines and provide a quick start to the experimental process especially for users that frequently use multiple XPS beamlines at MAX IV. The project is almost purely software in nature and has encountered some delays due to the different software demands from the two major XPS instrument providers (SPECS and Scienta) and difficulties integrating them into the MAX IV control and data acquisition system.

The ultimate aim of the project would be that a user coming to any of the MAX IV XPS beamlines would always be faced with a similar interface for acquiring electron spectra. This ambitious goal may of course not be fully achievable as beamlines are unique in certain situations. For example, acquiring ARPES often requires a rather different interface to acquiring time-resolved XPS in a gas environment. Therefore, the beamlines themselves are still in control over the type of acquisition program they will provide. In addition, the aim is to use already existing software infrastructure and backend capabilities at MAX IV in order to reach this goal. Most beamlines at MAX IV use a Sardana[29]-based acquisition and measurement orchestration service. Integrating the XPS acquisition into Sardana might cause additional unforeseen problems that require further work to fully resolve in a manner that ultimately produces a suitable measurement program. Another unresolved challenge is online data visualization (i.e. displaying the currently acquired spectra). For example, SpecsLab Prodigy (the XPS acquisition bundled together with all SPECS spectrometers) contains a large suite of analysis features which are quite mature and useful. Replicating all of this functionality by the MAX IV software group will require a lot of effort.

SPECIES has been a part of the project, but the project overall is coordinated at the facility level. It was recently decided that the part of the project dedicated to SPECS spectrometers should have a lower priority compared to Scienta so that the work on Scienta spectrometers would proceed faster. Therefore, from the point of view of the beamline, the work has essentially stalled for about six to nine months, but the work is expected to resume soon.

**Establishing equipment tracking and maintenance system**

MAX IV and the beamline are in the process of setting up a system for keeping track of all beamline equipment, instruments, spare parts, and various other components in a large-scale management software suite. This software is expected to streamline the various processes that are needed in order to keep all the beamline equipment maintained and in good working order for the foreseeable future. Currently, most

[29] https://www.sardana-controls.org/

maintenance tasks are organized in an ad hoc manner, which has serious drawbacks. An automated system with built-in functionality to assist the beamline staff in keeping track of various equipment and spare parts would free up valuable time currently spent in updating various Excel files. Establishing this system is expected to be rather important for the beamline. However, such a system requires a facility wide coordinated effort. Due to lack of resources, the lab has not been able to prioritize the development of this system and therefore it has been delayed significantly. The recent hiring of a development engineer is expected to accelerate the work. The beamline staff have only a small role in the project as a whole but the beamline has been offered as a testing platform in order to try out the new program and its features.

**New features of the APXPS endstation**

Sample transfer within the APXPS endstation is currently quite time-consuming. This mostly originates from the fact that all samples have to be loaded through the preparation chamber, which has a slow manipulator motor. It takes roughly 15 minutes to move a sample from the load-lock to the measurement chamber. When a user group comes with an experimental plan that involves a lot of sample exchanges or sample preparation which requires moving the sample between the analysis and preparation chambers, the time spent waiting for manipulator movements to finish can quickly grow to be substantial. To improve the efficiency of measurements and speed up the sample transfer, the manipulator could be upgraded to a faster version. At the same time, the manipulator motion control could be changed to the MAX IV standard IcePAP-type motor control scheme. In addition, the load lock chamber could be upgraded to be able to load more samples at a time. These two improvements would likely increase the utilization of beamtime and make the system more efficient and user friendly.

Currently, the upgrade of the preparation manipulator and the load lock chambers are in the planning stage. It is expected that the upgrade will be funded through MAX IV opportunities. However, the priority has not been set very high, and therefore so far not a lot of work has been allocated to the project. To push this forward, careful planning and analysis of available manipulator solutions should be carried out in order to come up with a budget estimate.

**Developing AP-XAS permanently for the RIXS endstation**

With the Italian AP-XAS collaboration (see section above about AP-XAS setup), a new avenue is opened up for the RIXS endstation. The sample rods could easily be further developed to have a dedicated sample environment for carrying out ambient pressure XAS measurements using the already available instrumentation at the RIXS endstation. This also opens up the possibility of doing RIXS measurements on high pressure systems, if that ever becomes a feasible avenue of research.

We see this development as a natural follow-up from the AP-XAS endstation collaboration. The SPECIES-RIXS endstation is a suitable place to house this sample environment and the beamline itself is well suited for studying many of these systems.

**Full upgrade of the APXPS endstation**

The APXPS endstation was originally procured from SPECS in 2010. At the time of writing this review, it is about 14 years old, which is starting to show in some areas. While several instruments have been upgraded over the years, it is still mostly the same vacuum chamber layout as was originally designed by SPECS. The current layout is very compact, but it poses some challenges especially in the way samples are transferred between the chambers. When compared to “modern” chamber layouts, it becomes evident that the layout at SPECIES is slightly outdated. The sample transfer is slightly clunky and difficult for new users to learn quickly enough to be comfortable using in one week of beamtime and requires several manual steps making it impossible to automate.

Therefore, in an attempt to dream big and bold, we are also proposing a completely new layout for the endstation. Exact details remain unsolved, but our aim would be to develop a new way of transferring samples from the load-lock into the AP cell which would be easier for users and possibly also motorized for additional automation.

Such drastic change to the beamline would also open the opportunity to re-design several other aspects, such as how the ambient pressure cells are introduced into the analysis chamber. One undesirable design choice, especially in the ALD cell, is the very long gas lines and the setup could be considerably improved by re-designing the way the gas lines are going into the cell. Similar changes could also be made for the other AP cells.

Currently, these long-term ideas are only in the planning stage. It is expected, however, that some upgrade of the endstation is required to keep the endstation productive and attractive to users while not falling behind any new trends in the APXPS community.

## 5.4 Prioritization of the development projects

Below we specify the prioritization of the various projects explained in detail above. The projects are given a priority number between 1 – 10, with 1 being the highest priority for implementation. When available, we detail here the funding and resources available for each project and their current status.

| Project | Priority | Funding and resources | Status |
|---|---|---|---|
| **APXPS gas system** | 1 | Funded by MAX IV. High amount of MAX IV and beamline resource needs. | In progress |
| **APXPS high temperature cell** | 1 | Externally funded (~2.2 MSEK). Mostly beamline resources. | In progress |
| **APXPS gas chromatograph** | 2 | Seeking external funding. Realized through mostly beamline resources | Awaiting funding |
| **AP-XAS project inclusion to RIXS endstation** | 2 | Funding acquisition ongoing. Uses mostly beamline resources | In progress |
| **New grating** | 2 | MAX IV funding and resources. | Pre-study started |
| **Continuous energy scanning** | 2 | MAX IV funding and resources. | Awaiting MAX IV resources |
| **User friendliness by automation (APXPS)** | 3 | Beamline and software group resources | Continuously on-going |
| **APXPS low temperature cell** | 3 | No funding yet. Uses beamline resources. | Not started |
| **Develop AP-XAS as permanently available technique** | 4 | No funding. Needs beamline and MAX IV resources. | Awaiting AP-XAS project conclusion |
| **APXPS new load-lock and preparation chambers** | 5 | No funding yet, needs high beamline resources. | Not started |
| **APXPS new TDC/detector maintenance** | 5 | No funding yet, uses mostly beamline resources. | Not started |
| **APXPS Spectrometer integration** | 6 | MAX IV funding. Needs mostly IT resources. | Awaiting MAX IV resources |
| **Establish maintenance system (J5)** | 7 | MAX IV funding and resources. | Awaiting MAX IV resources |

| | | | |
|---|---|---|---|
| **APXPS sulfur cell** | Pending feasibility | Has no external funding. Uses high beamline resources, (needs extra staff) | On-hold |

# 6 Points of concern

**Low energy RIXS**

The combination of the high flux at lower energies of the SPECIES beamline and a high transmission, high resolution instrument should be an excellent combination. The instrument was originally designed to study M-edges of the transition metals, but the near-absence of momentum transfer from the photons at these energies combined with the advent on large instruments with comparable absolute resolutions at the L-edges since the instrument's inception has impacted interest from the user community. However, there are possible other interests for this energy range. Lithium compounds for instance are notoriously difficult to study in XAS and RIXS and this instrument could fill this void. Other edges like the sulphur edge would also be of interest.

**High-energy RIXS**

At the higher energies the SPECIES beamline suffers from low flux for being of use for RIXS experiments. This severely lessens the attraction as a RIXS beamline for edges above the C K-edge. The instrument itself has some appeal with its larger energy window but as a whole one should consider how to make use of this energy range. For simple XAS measurement it is still viable both in TEY and TFY.

**Beamtime division between branches**

The allocated beamtime division between the branches has always favored the APXPS side. Some of this originates from the demand of user communities. For example, by comparing the number of submitted proposals to the branches (see Figure 22~~Figure 22~~), one can see that the demand for the RIXS endstation is not nearly as high as for the APXPS. However, if the demand from the RIXS community would suddenly increase (for example due to the PGS becoming more popular and productive) it would be challenging to decide where to put the beamtime focus.

An additional aspect to consider is also the development of the AP-XAS cell which is planned for installation and operation in the RIXS endstation and is going to take some of the beamtime dedicated for RIXS users. The decision about the operation of the AP-XAS cell was taken at a time when there was not so much information about the functionality of the PGS and therefore it was deemed more productive to place the AP-XAS developments at the same endstation.

Assuming the beamtime division needs to change in the future, it would of course be fruitful to make the decisions based on scientific excellence, i.e. only grant those proposals that produce high quality science. The judgement of high-quality science might be challenging to do as the comparison between APXPS (and AP-XAS) and RIXS is difficult due to the very different nature of the experiments and obtained results. A valid guideline for experiment selection is, however, given by the MAX IV strategy. There are also other minor changes that would need further reevaluation, for example the fact that the proposals for the two techniques are evaluated by two different committees. Therefore, for the short-term at least, the decision is to stick to similar beamtime division between the branches as it exists now, i.e. about 60/40 in favor of the APXPS endstation, which gives plenty of beamtime opportunities for APXPS users while still providing adequate RIXS beamtime for some users and in-house work.

**Low flux at high photon energies**

As mentioned above, the beamline has lower than expected flux at high photon energies of. There could be several reasons for this, ranging from carbon-contaminated optics to deteriorated Au coatings.

To address this problem, a new grating could be installed. Currently, the 1221 l/mm grating is used throughout the whole spectrum. Most likely another ruling density might suit higher energies better while sacrificing some of the resolution. This would benefit XPS users tremendously, as nearly all users need access to photon energies above 700 eV.

Currently, a project has been approved to begin a pre-study for the new grating (this was specified above in 5.2). The specifications (appropriate ruling density, blaze angles, etc.) are being simulated to find optimum conditions that would give the most benefit at these energies. For the grating targeting improved high-energy performance, we expect to gain an increased flux by about a factor of 2 (at energies above 400 eV). However, this depends heavily on the type of problem we are facing with the beamline. If the degradation mostly originates from the grating, then getting a new one might have a more dramatic effect on the flux increase.

Similar developments are being carried out at MaxPEEM and FlexPES beamlines, which are similar to SPECIES in the beamline flux curves. The increased flux at those beamlines has been seen as a very positive development.

## 6.1 Point of consideration: APXPS and RIXS activities across the lab

For APXPS, HIPPIE and SPECIES beamlines overlap a lot in terms of scientific areas in their respective user science programmes. This can be seen as being both positive and negative. Positive in a sense that there are plenty of opportunities for users to carry out their research since there is more beamtime available through two beamlines. But it can be negative, in areas where not so many users exist, and the beamlines might (unknowingly or unwillingly) compete against each other. This could ultimately lead to a decrease in scientific quality, as there is not so many opportunities to select good science anymore when the pool of proposed experiments becomes shallow.

In many areas, however, the beamlines differ substantially. For example, HIPPIE has a dedicated electrochemistry setup and SPECIES is focused on *operando* ALD studies, to name just two areas out of many. This can lead to a positive force, where the beamlines specialize in certain areas and can focus more on that while also having the possibility of offering unique tools for the user community to exploit for cutting edge research.

The scientific overlap between SPECIES and HIPPIE is therefore a complex question, but a point of concern exists. We do feel that the matter should be handled delicately in the future whenever the direction of the APXPS programme at MAX IV is considered. Especially interesting is the interest from other beamlines who are going into the direction of (near-)ambient pressure conditions in their respective XPS/XAS systems (these kinds of plans are in motion at the FlexPES and MaxPEEM beamlines). In addition, the current plans for building new dedicated hard X-ray instruments for APXPS should merit discussion about the direction of APXPS activities throughout the lab.

For RIXS activities similar considerations exist. They are, however, much less serious since the available energy ranges with good enough flux differ substantially between SPECIES and Veritas. The user community might have a different makeup than the APXPS community, questioning the need to have two very similar RIXS beamlines. Especially interesting is the necessity of even trying to offer high-energy RIXS at SPECIES when it is often very unproductive use of time.

# 7 Charge questions

1) Technical realization of the beamline:
    a. **Should SPECIES continue to offer low energy RIXS as a technique in the current landscape of available RIXS instruments?**

   i. Should SPECIES continue to offer RIXS at higher energies (>200 eV)? Should this type of work be concentrated at Veritas?
   ii. Is the development of the AP-XAS programme a valid direction for the RIXS endstation, even if it takes away some beamtime from purely RIXS research?
- **b. For APXPS: How high risk does the sulfur cell pose for contaminating the endstation and therefore rendering any further "clean" experiments impossible?**
- c. Does the beamline provide adequate capabilities, and does the beamline team address areas of necessary improvement?
- d. Does the beamline offer unique capabilities to the user community?
- e. How does the beamline compare to leading beamlines in its field worldwide?

2) User communities, science programme, and impact:
   - **a. Is the beamline attracting and supporting the relevant user communities?**
   - b. Do the capabilities meet the needs of the relevant scientific communities~~?~~
   - c. Are the staff research and development projects of appropriate quality and in line with the current and future direction of the science programme at the beamline?
   - d. Are user and in-house science programmes productive and making a sufficient impact in their science fields?
   - e. Is the beamline missing opportunities regarding user communities, science programmes, or research directions?
   - f. Does the beamline / MAX IV employ an adequate outreach and training programme?
3) Beamline operation:
   - **a. Is the user support at the beamline of high quality and allowing for a productive user programme with high impact?**
   - b. Is the beamline or the facility missing out on opportunities for further improving user productivity?
   - c. Is the facility setting the right priorities in providing high-quality supporting infrastructure (*e.g.* gas project), services, and procedures?
4) Future directions:
   - **a. Is the list of priorities realistic for the APXPS and RIXS teams?**
   - b. Does the beamline have a well-laid-out and actionable development plan?
   - c. With the user community and national and international developments in mind, are the right priorities set out for these developments?
   - d. Is the beamline / MAX IV having an adequate funding strategy and making use of funding opportunities?
   - e. Are there additional opportunities (funding, development, science directions) that the beamline or the facility should take into account?
   - f. Are the (envisioned) operation and science programmes at the beamline well-adjusted?