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TXPES – A new soft X-ray spectroscopy beamline at the SESAME synchrotron

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Abstract. The Turkish Soft X-ray Photoelectron Spectroscopy (TXPES) beamline project at the Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) synchrotron, led by Turkish Energy Nuclear and Mineral Research Agency (TENMAK) is an important development as it marks SESAME's first beamline fully designed, manufactured, and installed by a member country, Turkiye in 2025. TXPES will be installed on the free branch of the Helmholtz-SESAME Soft X-Ray Beamline (HESEB) and will share the same photon source and monochromator. The beamline will provide tunable photon energies ranging from 90 eV to 1800 eV for detailed analysis of the electronic structure and chemical bonding of materials. The end station supports techniques such as X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS) and Low-Energy Ion Scattering (LEIS), thanks to advanced tools like the PHOIBOS 150 Complementary Metal-Oxide-Semiconductor (CMOS) XPS/LEIS/UPS Analyzer. With its versatile design and High-Pressure Cell (HPC), the TXPES system offers exceptional surface sensitivity, spatial resolution, and energy resolution, making it ideal for interdisciplinary research in physics, chemistry, materials science, and engineering.

1. TXPES Beamline: Project Overview, Development, and Implementation Stages

SESAME is a 2.5 GeV third-generation synchrotron light source providing a broad range of radiation, from infrared to X-rays. In 2018, Deutsches Elektronen-Synchrotron (DESY), together with leading German research institutions—Helmholtz Zentrum Berlin (HZB), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Forschungszentrum Jülich (FZJ), and Karlsruhe Institute of Technology (KIT)—collaborated to establish the HESEB beamline at SESAME. HESEB includes a free branch for the addition of another end station and photon beamline. Building upon the established framework of the HESEB beamline, Turkiye is contributing by manufacturing an additional beamline branch. The TXPES project aims to construct an X-ray optics transport line and a Soft X-ray Photoelectron Spectroscopy end station at SESAME, complementing HESEB. This marks the first beamline designed, manufactured, and installed by a SESAME member country, Turkiye. The TXPES project, led by TENMAK, is a collaborative effort involving Bilkent University, Koç University, and the Turkish Accelerator and Radiation Laboratory (TARLA) in Turkiye. The Helmholtz Association has significantly contributed to the project by constructing the X-ray transport optics line, essential for directing synchrotron radiation to the beamline. This initiative aims to establish a soft X-ray spectroscopy beamline branch that will share the same undulator and monochromator as the HESEB beamline. Complementing this new branch will be a multi-functional surface characterization end station, designed to offer advanced analytical capabilities for studying surface properties.

The TXPES beamline construction, initiated in 2022, is progressing with two main work packages: TARLA's design and manufacturing of the X-ray optics transfer ultra-high vacuum (UHV) line, and Koç University and Bilkent University's design and construction of the XPS experimental end station, in partnership with SPECS GmbH of Berlin. Once completed in 2025, the TXPES beamline will facilitate advanced surface-sensitive XPS measurements, providing valuable insights regarding the electronic structures, elemental composition, oxidation states, depth profiling and surface chemistry of a large variety of advanced materials. It will support research on nanomaterials, catalysts, thin films, electronic materials, sensors, and batteries, advancing fields such as energy conversion, energy storage, catalysis, renewable energy systems, optoelectronics, photonics, and environmental science.

2. Beamline Technical Overview

The TXPES beamline will utilize the same photon source and monochromator as HESEB and will be located directly adjacent to the HESEB beamline. The optical layouts for both beamlines are provided in the HESEB technical paper [1].

2.1 Photon Source and Monochromator

- APPLE II Undulator: The 1.7-meter-long APPLE II undulator, with 30 periods of 56 mm each, provides precise polarization control for circular and linear polarization. It covers a photon energy range of 90 eV to 1800 eV, enabling TXPES to study various elements and chemical states.
- Collimated Plane Grating Monochromator (PGM): TXPES is equipped with a PGM that has two gratings (400 and 1200 grooves/mm ensures precise photon energy control and optimized flux, producing a beam spot size of 180×25 μm^2 for high-resolution surface studies. Detailed information on the undulator and monochromator can be found in references [1,2].

2.2 Beamline Optics and Components

- Beam Splitter Unit: Positioned immediately after the PGM, toroidal M3ab mirror enables the division of the photon beam, allowing both the HESEB (ID11-left) and the TXPES (ID11-Right) branches to operate interchangeably (Figure 1). This versatility ensures that the beamline can accommodate various experimental setups and user requirements.
- Optics Configuration: The optical branch line of TXPES will consist of a Horizontally defining slit (HDS), a Vertically defining slit (VDS) or Energy slit, an M4b Mirror system, and an End Station (Figure 2). The HDS is designed to define the horizontal dimension of the beam, featuring two independent actuators that facilitate an opening range from 5 mm to 20 mm. The system is equipped with a beam monitoring capability, utilizing a Yttrium Aluminum Garnet (YAG) screen

coupled with an attached Charge-Coupled Device (CCD) camera to provide real-time observation and measurement of the beam profile.

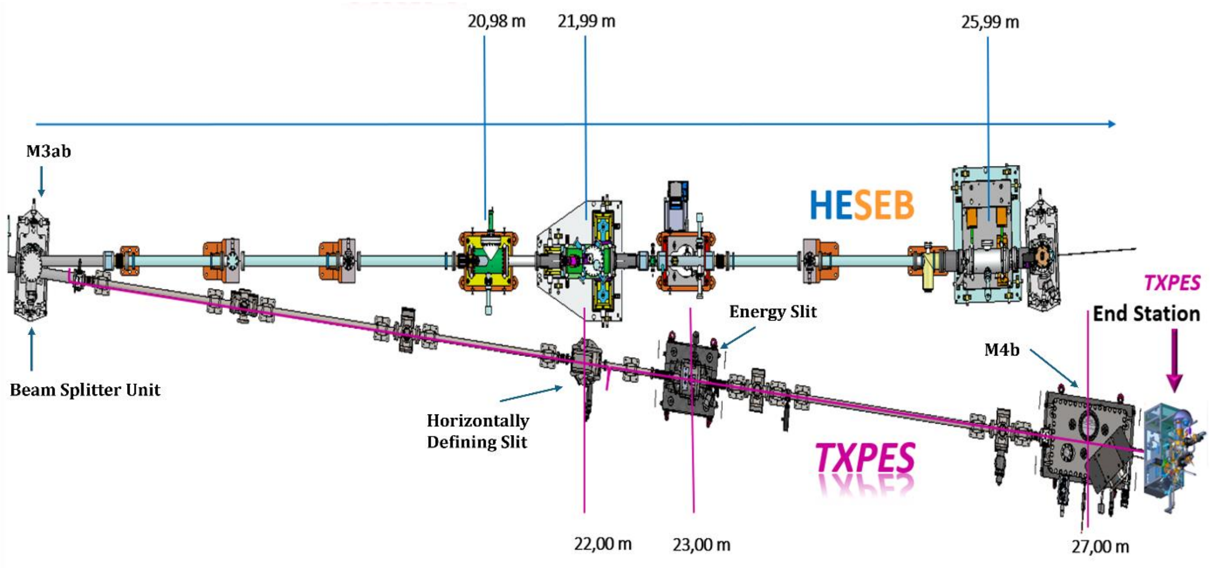


Figure 1. TXPES Beamline: Schematic Layout.

The VDS or energy slit unit defines the vertical beam dimension, impacting energy selection and experimental results. To ensure precision, a blade alignment system with encoders placed close to the blades achieves 50 nm accuracy. The system also features two actuators for gap translation and uses innovative internal mechanics for optimal performance (For the HDS and VDS configurations, see Figure 3).

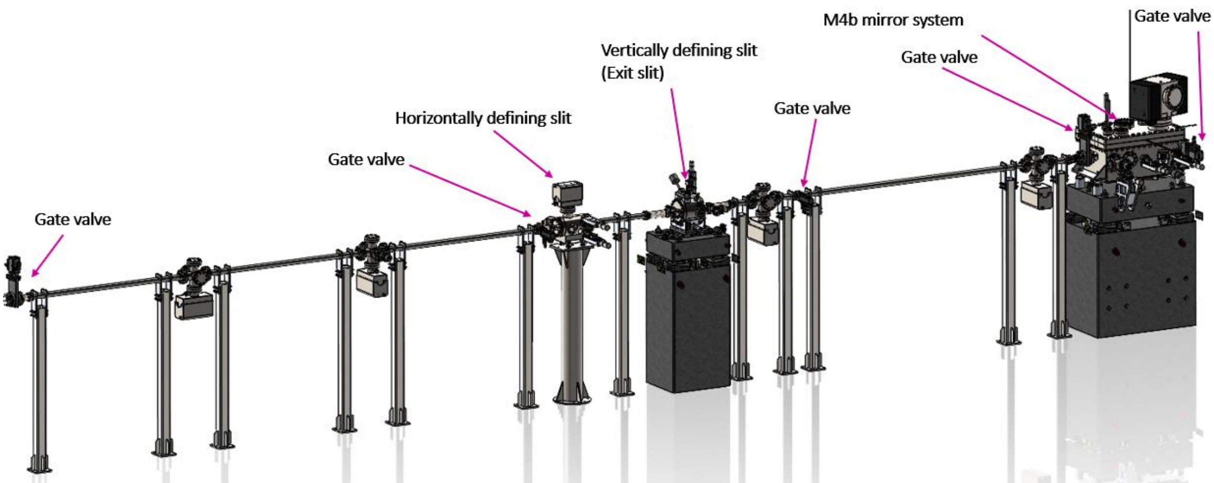
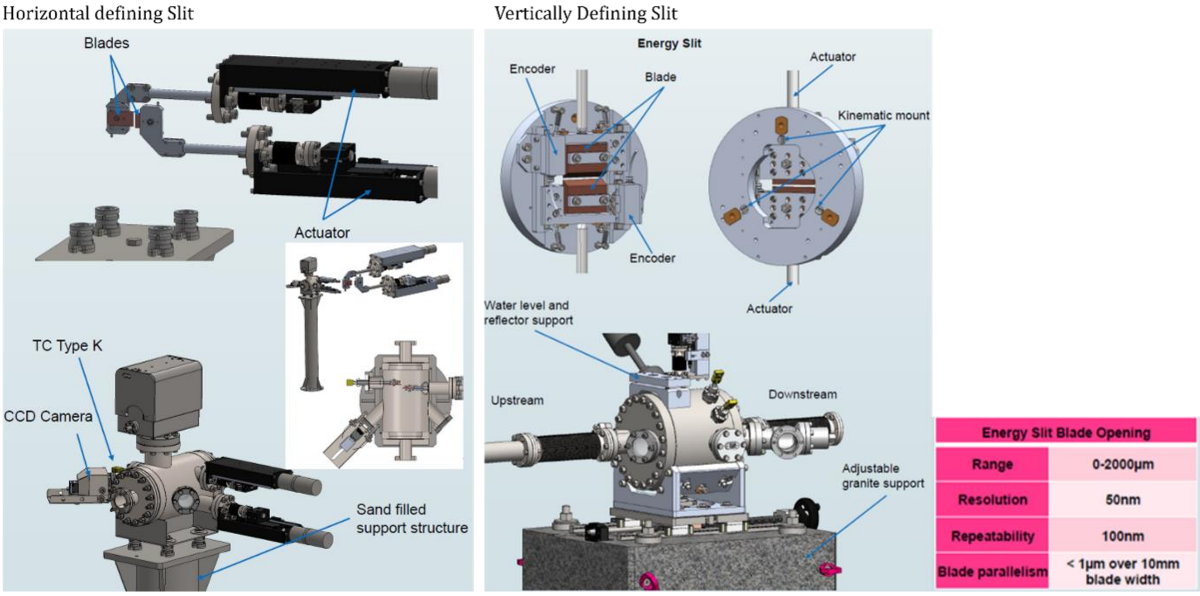


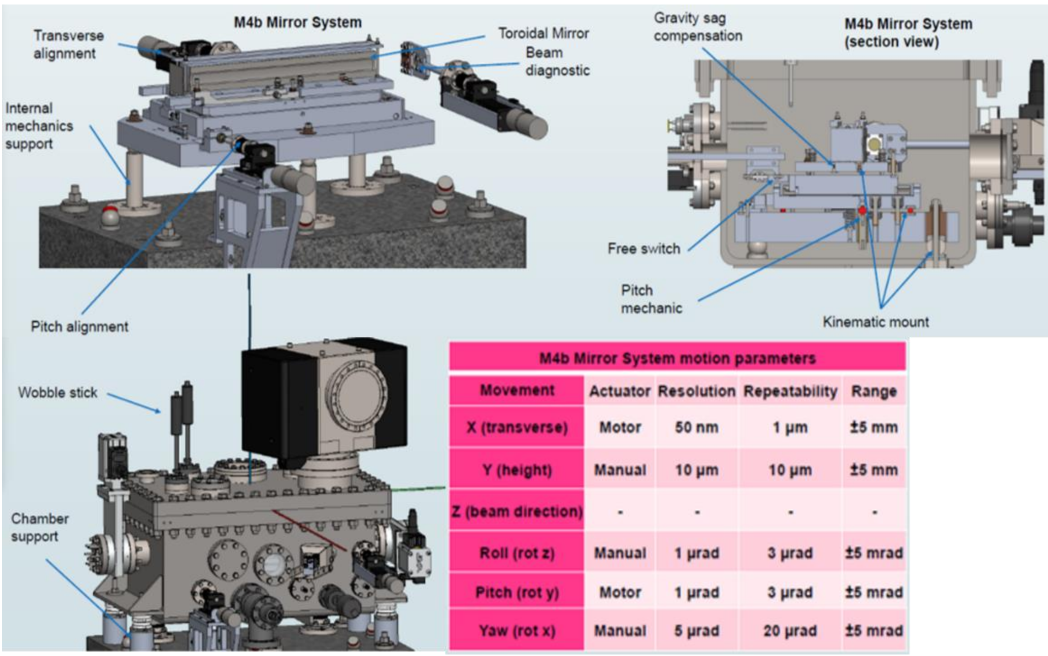
Figure 2. X-ray Transfer Optics branch line components of the TXPES beamline, designed to optimize beam delivery and enhance analytical precision.



Energy Slit Blade Opening	
Range	0-2000µm
Resolution	50nm
Repeatability	100nm
Blade parallelism	< 1µm over 10mm blade width

Figure 3. Horizontal and Vertical Defining Slit: Schematic and Parameters.

The refocussing M4b toroidal mirror system is equipped with two motorized and three manually adjustable alignment axes, providing precise control over mirror positioning. It features a force-free mounting design to avoid any deformation caused by the mounting process, ensuring stability and accuracy from the base plate to the mirror holder. To mitigate errors induced by gravity, the system includes spring-loaded supports that are electrically insulated, maintaining the mirror's alignment and performance. This combination of features ensures that the mirror operates with high precision and minimal interference from external forces (Figure 4).



M4b Mirror System motion parameters				
Movement	Actuator	Resolution	Repeatability	Range
X (transverse)	Motor	50 nm	1 µm	±5 mm
Y (height)	Manual	10 µm	10 µm	±5 mm
Z (beam direction)	-	-	-	-
Roll (rot z)	Manual	1 µrad	3 µrad	±5 mrad
Pitch (rot y)	Motor	1 µrad	3 µrad	±5 mrad
Yaw (rot x)	Manual	5 µrad	20 µrad	±5 mrad

Figure 4. M4b Toroidal Mirror Unit System: Schematic and Parameters.

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The UHV and optical components of TXPES beamline have been manufactured in Turkiye, except for the toroidal mirror of the M4b unit, which was ordered from Carl Zeiss GmbH (Germany). The Factory Acceptance Test (FAT) for the mirror was successfully completed. FAT for the remaining components is scheduled for later in 2024, ensuring that all parts meet the required technical specifications. All chambers have passed leak testing, and components are cleaned and ready. Assembly has begun, with installation at SESAME by TARLA expected to start in early 2025.

3. TXPES End Station Design and Instrumentation

The TXPES End Station is a state-of-the-art facility designed to deliver comprehensive surface and interface characterization, focusing on the advanced analysis of materials within a synchrotron environment. It consists of four main chambers, as illustrated in Figure 5, each serving a crucial function in material characterization and surface science research:

1. Analysis Chamber: The Analysis Chamber is equipped with advanced instrumentation designed to achieve high-resolution surface and interface characterization. At its core, the PHOIBOS 150 CMOS Analyzer provides detailed chemical and electronic structure analysis through XPS, UPS, and LEIS offering exceptional spatial and energy resolution for examining elemental composition and chemical states at the atomic level. The XR 50 Dual Anode X-ray Source supplies X-rays crucial for XPS, facilitating low-resolution XPS analysis during the maintanance periods where syncrothron radiation is not available. For UPS, the UVS 10 ultraviolet (UV) source enables comprehensive studies of electronic structures, including valence band characterization and work function determination. In addition to XPS and UPS, Angle-Resolved Photoemission Spectroscopy (ARPES) enriches material analysis by mapping electronic band structures, providing critical insights into complex materials such as topological insulators, superconductors, and 2D materials. An electron flood gun is employed to neutralize surface charge accumulation during XPS measurements, ensuring accuracy and stability, especially for insulating materials. The rastering ion gun allows precise LEIS analysis and XPS depth profiling, enabling the removal of surface layers for elemental analysis at varying depths. Additionally, the 4-Axis sample manipulator provides precise sample positioning with liquid nitrogen cooling down to below 100 K and e-beam heating up to 1200 K, making it essential for conducting temperature-dependent studies, such as catalytic reactions or phase transitions.

2. High-Pressure Chamber: The high pressure chamber is a unique component of the end station that mimics real-world catalytic conditions, enabling sample treatments at high pressures and temperatures. HPC-20 allows reactive sample pretreatment under conditions of up to 10 bar and 800 °C, making it ideal for catalysis and material science studies involving gas-solid interactions under near-operational conditions.

3. Preparation Chamber: The preparation chamber is equipped with a comprehensive array of tools designed for sample preparation, modification, and treatment. The ion gun for sputtering is used to remove surface contaminants such as oxides and adsorbates, ensuring clean surfaces for accurate analysis. The radio frequency (RF)-plasma source facilitates plasma treatment for surface modification, essential for cleaning, activating surfaces, and preparing them for thin-film growth or other treatments. Low-Energy Electron Diffraction (LEED) provides insights into surface crystallography and structural properties, crucial for understanding surface reconstructions. The Quadrupole Mass Spectrometer (QMS) performs residual gas analysis (RGA), monitoring residual gases to maintain UHV conditions and also enables leak check for the UHV system. Metal/metal oxide evaporators enable in situ thin-film deposition, allowing well-controlled material interfaces and investigations regarding thin-film growth dynamics. Gas dosers allow precise introduction of reactive gases for catalysis research and surface reactions, while the 4-Axis Manipulator offers liquid nitrogen cooling down to below 100 K and e-beam heating up to 1200 K, ensuring optimal sample positioning and temperature control for diverse experimental setups.

4. Load Lock Chamber: The Load Lock Chamber is designed for rapid, contamination-free sample exchange, allowing samples to be loaded and removed under vacuum conditions, minimizing downtime and preventing degradation during the exchange process.

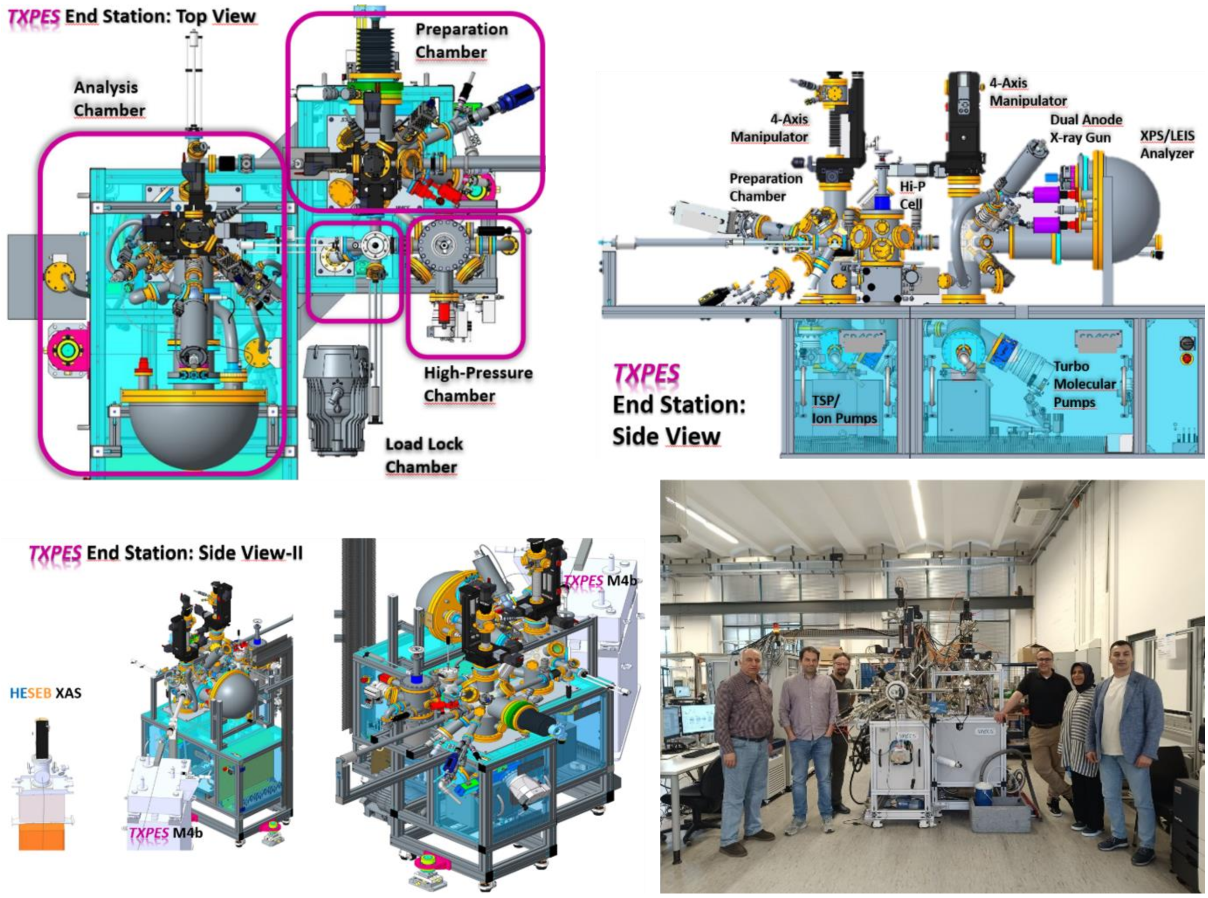

Figure 5. TXPES End Station: Top and side schematics and a photograph from the FAT in Germany.

The FAT for the TXPES End Station was successfully completed at SPECS in Berlin during the first half of 2024, with installation at SESAME scheduled for late 2024. The integration of the end station into the TXPES beamline is expected to be completed by early 2025. Commissioning is anticipated to conclude by spring 2025, with the beamline projected to be ready for user operation by the second half of 2025. The TXPES beamline will enable precise identification of elements (excluding hydrogen and helium) and accurate composition determination, with high brightness improving the signal-to-noise ratio and thus reducing data acquisition times. Tunable photon energy supports high-resolution spectroscopy, elemental mapping, and detailed depth profiling, while high spatial resolution and reduced photoionization cross sections at higher energies enhance accuracy in surface and near-surface composition analysis.

References

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[2] Follath R and Friedmar S 1997 *Nucl. Instrum. and Methods* **A390** 388-394