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# PEAXIS: A RIXS and XPS Endstation for Solid-State Quantum and Energy Materials at BESSY II

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**Abstract:** PEAXIS (Photo Electron Analysis and resonant X-ray Inelastic Spectroscopy) is a dedicated endstation installed at the beamline U41-PEAXIS that offers high resolution soft X-ray spectroscopy measurements with incident photon energies ranging from 180 – 1600 eV. The endstation combines two X-ray spectroscopic techniques, X-ray photoelectron spectroscopy (XPS) and resonant inelastic soft X-ray scattering (RIXS), which are important for probing the electronic structure and local and collective excitations of solid-state materials. It features a continuous variation of scattering angle under UHV conditions for wave vector-resolved studies and a modular sample environment that allows investigation in the temperature range between 10 K and 1000 K.

#### 1 Introduction

The electronic structure and dynamics of materials determine their fundamental and functional properties which are relevant for technological applications. PEAXIS (Photo Electron Analysis and resonant X-ray Inelastic Spectroscopy) offers the possibility of probing electronic states of materials by two sought-after X-ray spectroscopic techniques in one single instrument. The instrument is designed for studying solid-state materials by Resonant Inelastic X-ray Scattering (RIXS) and X-ray Photoelectron Spectroscopy (XPS) and, in addition, allows for the investigation of liquids encapsulated in a sealed

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cell. The fixed endstation is installed at the beamline U41-PEAXIS of BESSY II providing monochromatic, linearly polarized light. The endstation allows for measurements with high energy resolution in combination with a continuous rotation of its 5 m long arm about the sample position. Scattering angles from 33°-139° are thus covered within the horizontal photon scattering plane which enables wavevector-resolved measurements of solid-state samples over a wide wavevector range and, with PEAXIS' sample manipulators, covering a temperature range from 10 - 1000 K. For sensitive samples, a continuous sample scanning mode is available in order to take measurements with minimal exposure time per surface area while keeping the scattering conditions constant. The instrument is also capable of performing angle-resolved XPS measurements thus allowing to probe the electronic structure of material from surface to bulk. In-house developed software (Centralized Hardware-Overseeing Server, CHaOS and Augmented Data Loading Evaluation Reduction, ADLER) is available to remotely control the experiment and perform a first-level analysis of the raw data. This allows users to have real-time feedback on the acquired data that is critical for remote-access experiments.

## 2 Instrument applications

Typical applications:

- Magnetic, d-d and charge transfer excitations in model quantum materials and functional energy materials
- Dispersive excitations in quantum materials (e.g. plasmons and excitons)
- Electron-phonon coupling in solid-state materials
- Reaction mechanisms in battery materials



## 3 Technical data

Source	Undulator U41	Horizontal polarization
Monochromator	800 l/mm PGM	
Energy range	180 - 1600 eV (XPS),	
	200 – 1200 eV (RIXS)	
Energy resolution/	311 meV - 24 meV / 3850 - 8250	High-flux (Cff = 2.25, slit = 20 μm)
Resolving power	231 meV - 21 meV / 5200 - 9750	Standard (Cff = 3, slit = 10 μm)
	200 meV - 15 meV / 6000 - 13600	High-resolution (Cff = 5, slit = 5 $\mu$ m)
Flux at sample	$1.4 \times 10^{11} - 4 \times 10^{12} \text{ s}^{-1}$	High-flux mode (@N2 resonance E)
	$(5.7 \times 10^{12} \text{ (s}^{-1} \times 0.1\% \text{ BW x } 100 \text{ mA}))$	
Focus at sample	12.4 x 3.8 μm <sup>2</sup> (hor. x vert.)	
Sample size	< 10 x 10 mm <sup>2</sup> , thickness $\sim$ 1.5 mm	
Sample	10 - 330 K (closed cycle refrigerator)	Low-T manipulator (solid samples)
environment	77 - 1000 K (with special holder)	High-T manipulator (solid samples)
	77 - 370 K	Fluid cell (liquid samples)
Pressure	$10^{-8} - 10^{-9}$ mbar	Regular operation
Sample movement	Static, 0.05 mm/s, 0.1 mm/s, 0.2 mm/s	
speed		
Number of samples	6	At load-lock
Sample treatment	Ar sputtering, annealing, cleaving	At load-lock
Optics	2 VLS gratings	200 - 600 eV and 400 - 1200 eV
Detectors	Andor IKON-L CCD 2048 x 2048 pixels with	RIXS
	pixel size of 13.5 x 13.5 $\mu$ m <sup>2</sup>	
	SPECS Phoibos 150 EP	XPS
	Photodiode or sample current	XAS
Beam availability	12 h/day in units of 1 week	

Table 1: Technical data of beamline U41-PEAXIS and PEAXIS endstation



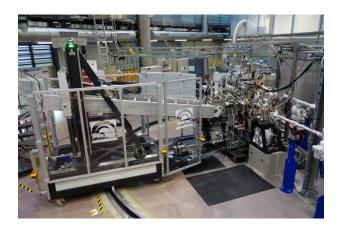


Figure 1: View of the PEAXIS endstation.

### 4 Acknowledgements

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#### References

Lieutenant, K., Hofmann, T., Schulz, C., Yablonskikh, M., Habicht, K., & Aziz, E. F. (2016). Design Concept of the High-Resolution End-station PEAXIS at BESSY II: Wide-Q-Range RIXS and XPS Measurements on Solids, Solutions, and Interfaces. *J. El. Spec. Rel. Phen.*. http://dx.doi.org/10.1016/j.elspec.2015.08.009

Lieutenant, K., Hofmann, T., Zendler, C., Schulz, C., Aziz, E. F., & Habicht, K. (2016). Numerical optimization of a RIXS spectrometer using raytracing simulations. *Journal of Physics: Conference Series*. http://dx.doi.org/10.1088/1742-6596/738/1/012104

Schulz, C., Lieutenant, K., Xiao, J., Hofmann, T., Wong, D., & Habicht, K. (2020). Characterization of the soft X-ray spectrometer PEAXIS at BESSY II. *J. Synchrotron Rad.*. http://dx.doi.org/10.1107/S1600577519014887

