

AI-XPRESS

AI-XPRESS is designed to transform materials discovery and optimisation. Bridging the gap between fundamental research and industrial application, its core capability lies in a fully integrated, roboticised, and AI-orchestrated environment for autonomous experimentation. The beamline will integrate a comprehensive suite of techniques—including XRD, XAS, XES, SAXS, WAXS, and anomalous scattering—across a 2–40 keV energy range, coupled with fast-scanning monochromators and advanced *in situ/operando* environments. The central vision is a self-driving X-ray laboratory where AI agents manage everything from robotic sample handling and real-time data reduction to hypothesis generation, using X-ray data as a "reward signal" for the AI-driven optimisation of material synthesis. Main scientific objectives include high-throughput spectroscopy and scattering, focusing on applied and industrial research in photovoltaics, catalysis, and advanced materials science. This setup aims to provide rapid feedback to improve processing and device operation at higher TRL levels. AI-XPRESS will capitalise on BESSY III's high flux from a high-field bending magnet source and the flexibility of its greenfield construction, fostering strong links with campus research.

Instrument	AI-XPRESS (<i>Autonomous Industry X-ray PROcessing, Efficient Scattering and Spectroscopy</i>)
Contact	Albert Gili de Villasante (albert.gili@helmholtz-berlin.de)
Source(s)	3T dipole (2-40 keV)
Beamline capabilities	Hutch 1 (MAP): • Energy range: 2-40 keV (all in chamber) • Resolving power: 7000 to 30000 • Spot size: >10x10 μm^2 (flexible using bendable KB mirrors) • Flux: up to 10^{11} ph/s Hutch 2 (FLOW): • Energy range: 2-40 keV (no fixed vacuum chamber, also in air) • Resolving power: 7000 to 30000 • Spot size: option for sub-micron focus • Flux: up to 10^{11} ph/s
Techniques	• (Grazing-incidence) XRD, SAXS, WAXS • (Grazing-incidence) XAS, XES, anomalous scattering (simultaneous XAS and XRD) • Quick XAS: ca. 1-3 ms for XANES and 10-100 ms for full EXAFS scans covering more than 1 keV scan range
Sample environment	Hutch 1 (MAP): • Self-driving lab with vacuum thin-film deposition & ambient wet chemistry, roboticised sample transfer Hutch 2 (FLOW): • Standardized <i>in situ/operando</i> gas reactors, cells, etc. • Materials hotel for long-term studies • Automated reactive processing suites (coating, sputtering, printing) • Possibility for "roll-in/roll-out" endstations