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UC6: Soft Matter and Liquid Interfaces X-ray Reflectivity Diffraction & Spectroscopy

Monday 24 March 2025 15:25 (7 minutes)

Within the soft matter and liquid interfaces X-ray reflectivity Use Case 6, we develop a FAIR data pipeline for X-ray reflectivity at beamline P08, PETRA III. This includes automating electronic lab notebooks (ELNs) [1], metadata ingestion from the control system and IGSN creation for samples. Collaborating with DESY beamline scientists, experimental control group, and IT, we are implementing automated metadata ingestion into SciCat, based on the proposed DAPHNE4NFDI metadata schema [2]. Here, we will present the current status of the data and metadata integration and the recently introduced PaN Reflectivity Database [3,4], aggregating high-quality photon and neutron reflectometry data. Additionally, we will show integration of machine learning solutions [5,6,7] for X-ray and neutron reflectometry, collaborating with large-scale facilities to including also for feedback to the instruments, including so-called closed loop experiments [8] and expanding research to include hard materials and magnetism.

References

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