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PolSpecX: Simulation and Analysis Tool for Polarised X-Ray Absorption Spectroscopy

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PolSpecX [1] is an integrated software tool designed for the simulation and analysis of X-ray magnetic circular dichroism (XMCD) and X-ray magnetic linear dichroism (XMLD) spectra of 3d transition metal elements at the L_2 and L_3 absorption edges. Leveraging the capabilities of Quanty [2-4] for multiplet calculations, PolSpecX enables accurate theoretical modelling of dichroic spectra under various electronic and magnetic configurations. In parallel, the tool provides a robust framework for the analysis of experimental data acquired from the magnetic materials beamlines at Diamond Light Source [5], or in principle any beamline using the NeXus file definition. Key features include automated subtraction of polarized spectra, background correction, application of XMCD sum rules for quantitative magnetic moment extraction, and direct comparison between simulated and measured spectra. By bridging advanced theoretical simulations with high-quality synchrotron data analysis, PolSpecX offers a comprehensive platform for researchers investigating the electronic and magnetic properties of correlated electron systems. Such a platform will enable visiting scientists to quickly assess the quality of their data and concentrate on the scientific goals of their beamtime.

Here we will show the web-based interface, explain the user-friendly design choices and highlight some preliminary comparisons between beamline data and simulation.

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