Contribution ID: **32** Type: **Oral Presentation**

Machine Learning for X-ray Spectroscopy: Hero or Zero?

Monday 5 January 2026 13:30 (40 minutes)

X-ray spectroscopy (XS) is undergoing such a transformation, powered by next-generation, high-brilliance light sources. As experimental capability expands, a new challenge emerges: How can we efficiently and accurately analyse the resulting data so that the rich quantitative information encoded in each spectrum is fully exploited? Extracting such insight increasingly requires sophisticated theoretical modelling to connect spectral signatures to underlying structure and dynamics, yet these calculations remain computationally demanding and technically complex.
In this talk, I will present our recent progress in addressing this challenge using supervised machine-learning and deep-learning approaches to predict X-ray absorption near-edge structure (XANES) spectra directly from local geometric information around the absorbing atom. We demonstrate that these models achieve sub-eV accuracy in peak positions and predict peak intensities with errors more than an order of magnitude smaller than the intrinsic spectral variations they are trained to capture. I will discuss the model architecture, its physical underpinnings, and its application across multiple absorption edges, highlighting how data-driven approaches can accelerate spectral analysis and broaden the impact of modern X-ray spectroscopy.

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Session Classification: Machine Learning for XAS Prediction and Analysis