Contribution ID: **12**

Type: **Poster and Flash Presentation**

A Bayesian Framework for Feature Extraction in Noisy Operando X-ray Absorption Spectroscopy

Monday 5 January 2026 16:38 (3 minutes)

We present a Bayesian framework for robustly extracting spectroscopic features from X-ray Absorption Spectroscopy measurements and synthetic reference datasets. This approach is particularly designed for complex XAS experiments with noisy spectra and irregular backgrounds, especially under operando conditions in the soft X-ray regime, where absorption by membranes in the optical path, sample environments and/or biased sample often compromises signal quality. Accurate identification of overlapping signal peaks and separation from experimental background and noise is crucial for interpreting fine structural and electronic information. Our approach combines physics-informed forward models for background, absorption edge, and composite peak shapes with Markov Chain Monte Carlo sampling to perform full posterior inference over model parameters. Using both laboratory-collected XAS spectra and controlled synthetic datasets, we show that the method can recover peak positions, widths, and absorption parameters for a broad range of spectra. We validate the pipeline by (i) recovering fiducial parameters from synthetic spectra, (ii) estimating dependence on experimental noise and parameter degeneracies using synthetic datasets, and (iii) producing posterior predictive checks showing agreement between data and reconstructed models. The implementation is computationally efficient and supports parallel MCMC sampling; results include best-fit parameter estimates, marginalized posterior distributions, and diagnostic outputs for residuals and chi-squared statistics. This probabilistic workflow facilitates rigorous interpretation of XAS features and provides a generalizable tool for spectroscopic analysis where signal-background disentanglement and uncertainty quantification are required.

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Session Classification: Flash Presentations