Contribution ID: **3** Type: **Contributed Talk (≈20 minutes)**

X-ray Emission Spectroscopy for Real-Time Diagnostics in SFX experiments: A Machine Learning Approach

X-ray emission spectroscopy (XES) complements structural techniques like serial femtosecond crystallography (SFX) by providing insights into the electronic states at specific sites within a sample. At X-ray free-electron lasers, simultaneous SFX and XES measurements using a single pulse have already been performed —such as the determination of the oxidation states in metalloproteins. By using non-thermal plasma simulations alongside relativistic atomic data, we trained a neural network on synthetic XES data from protein crystals to predict fluence and pulse duration of the beam. Trained on synthetic data generated by a collisional radiative model, the network accurately predicts fluence with <1.5% relative error and when predicting both parameters concurrently with <12% error. Feature importance analyses reveal spectral regions tied to underlying physical mechanisms. The model emphasizes K to L shifts to higher emission energies due to presence of highly charged sulfur ions. This approach performs comparably to, and in some cases better than, current experimental setups that rely mainly on upstream X-ray gas monitors (XGMs). It offers a promising route toward real-time, high-repetition-rate diagnostics, effectively complementing existing XFEL beam characterization methods.

Scholarship elegibility

no

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