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Challenges and opportunities for machine learning in XAS data interpretation

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The last decade witnessed rapid development in data science and machine learning (ML) methods, which are finding more and more applications across diverse fields, and make a dramatic impact also on the processing of spectroscopic data. In particular, the application of unsupervised and supervised ML methods provides new opportunities for detecting subtle fingerprints of structural changes in working functional materials, processing large data sets from time- and spatially-resolved measurements, and could provide the key also for decoding multimodal spectroscopic data. The deeper integration of the ML into the various steps of data processing pipeline, starting from the first on-the-fly analysis carried out already at the next generation of beamlines, seems to be an imminent future. In this talk we will highlight the need for advanced XAS data analysis approaches, emphasizing the areas where ML could provide a viable solution, and illustrate it with a few recent examples of ML-based operando XAS studies of working electrocatalysts. Nonetheless, as highlighted in this talk, the interpretation of spectroscopic data for realistic functional materials under actual working conditions requires caution, regardless of the data analysis approach implemented. In particular, such materials commonly are mixtures of different species (e.g., passive spectators coexisting with active species), which poses a challenge for such sample-averaging methods as XAS, requiring special care and development of dedicated data analysis tools.

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