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Convolutional AutoEncoder for Anomaly Detection and Chemical-State Identification of XAS Spectra in Operando Catalysis

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Machine Learning (ML) techniques offer powerful tools for advancing scientific discoveries and are increasingly integrated into material science, particularly X-ray Absorption Spectroscopy (XAS) studies in situ. These methods enable applications ranging from real-time spectral analysis during catalytic reaction to the prediction of structural parameters [1,2]. As a wide range of spectroscopic data becomes accessible, data-driven and ML-based approaches gain more attention along grounded theoretical methods [3,4].
In the Helmholtz-funded ROCK-IT (Remote, Operando Controlled, Knowledge-driven, and IT-based) project [5], which aims to automate Operando Catalysis experiments at synchrotron light sources, high-quality XAS data were acquired for modeling X-ray absorption spectra, as demonstrated on CO_2 methanation using various catalysts. For the analysis of these experimental data, we utilized Unsupervised Learning methods, specifically Convolutional AutoEncoder (CAE) for XAS spectral Reconstruction and Anomaly Detection for data quality improvement, in addition to Chemical-state Identification over time through latent-space analysis [6,7]. AutoEncoders are neural network architectures designed to learn compressed representation of high-dimensional input data through Encoding/Decoding processes [8]. The Convolutional Neural Network (CNN) forms the basis for many image processing frameworks, adapted in this work for spectral analysis to learn spatial properties, extract relevant features, and identify anomalies within the spectral domain.

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