Analysing *operando* spectroscopy data in battery studies: a chemometric approach

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Abstract:
In the last decade, a growing number of *operando* spectroscopy analyses have helped unraveling the electrochemical mechanism of lithium and post-lithium battery materials. The corresponding experiments usually lead to very large amounts of data, which require a long and time consuming analysis, and are thus difficult to analyze thoroughly. An alternative and innovating approach to extract all possible information from such data is the use of chemometric tools such as Principal Component Analysis (PCA) and multivariate curve resolution (MCR).[1,2]
PCA is generally used to discover the minimal particular structures in multivariate spectral data sets. In the case of *operando* spectroscopy data, it can be used to determine the number of independent components contributing to a complete series of collected spectra during electrochemical cycling. The number of principal components determined by PCA can then be used as the basis for MCR analysis,[3,4] which allows the stepwise reconstruction of the "real" spectral components. A detailed description of this method from a theoretical point of view was given by Tauler et al.[1,5] who also proposed this method for the analysis of *in situ* spectroscopic data. The intrinsic limits of this method and of its application are discussed by Ruckebush et al.[6]
In this presentation, we will show how such approach can be effectively applied to different techniques, such as Mössbauer spectroscopy, X-ray absorption spectroscopy or transmission soft X-ray microscopy, for the comprehension of the electrochemical mechanisms in battery studies.

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Contribution: Invited