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POS-24 Applying State-of-the-art Machine Learning Methods to Analyse Electrolyte composition of Lithium-ion Cells using Fourier-Transform Infrared Spectroscopy

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Lithium-ion cells are complex electrochemical system and various physical properties can be measured, giving valuable insights into their behavior, state-of-health, degradation mechanisms, etc.. However, many such insights remain unexploited because of the difficulty of relating the raw data to the variables of interest. This is a setting well suited to Machine Learning. This talk will take as example the task of determining the composition of an unknown electrolyte, simply by using the Fourier-Transform Infrared (FTIR) spectrum. Some samples of known composition were measured, to build a calibration set, which was used to approximate the relationship between FTIR spectrum and electrolyte concentration.
Machine Learning methods have made significant leaps forward in recent years, achieving impressing results in image recognition, audio signal analysis, natural language processing, and even video game artificial intelligence. State-of-the-art methods in this emerging field of "deep learning"are however known to require huge amounts of data to achieve good results. This talk will demonstrate that this need not be so, by presenting a successful application of state-of-the-art complex neural networks to the problem of electrolyte analysis. A special emphasis will be given to the techniques developed to ensure the robustness of the resulting model, allowing the application of these techniques to more problems in the future. The resulting model will be compared to alternative techniques such as inductively coupled plasma optical emission spectrometry (ICP-OES) and Gas chromatography–mass spectrometry (GC-MS), thus validating it as a tool for the analysis of electrolytes from aged Lithium-ion cells, requiring no special sample preparation and using no harsh or expensive solutions.

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