Contribution ID : **28** Type : **Talk**

Automated Analysis of Neutron Reflection Data from a Lithium-Mediated Nitrogen Reduction Reaction Using Bayesian Evidence

Wednesday, 6 November 2024 10:40 (20)

Ammonia has been identified as a carbon-free energy vector with the potential to fill some of the void to be left in the energy landscape as the planet decarbonises. To aid in the chances of an ammonia fuel being implemented, new and scalable production processes are being studied to enable its synthesis at off grid renewable energy farms. Currently, the most viable method is the electrochemical-lithium-mediated nitrogen reduction reaction. The reaction works *via* lithium reduction at the surface of the electrode. The lithium then follows thermodynamically feasible reactions with dinitrogen to lithium nitride and with any labile protons in the system to produce ammonia. Despite this simple theory behind which the ammonia is formed the actual composition and morphology of the surface deposit undergoing the reaction is not known. The reaction's complexity is increased by the presence of a solid electrolyte interphase, produced by the decomposition of electrolyte species either electrochemically or upon interaction with reactive lithium species. The interphase is responsible for allowing uniform lithium plating and moderating in the influx of reactants at appropriate ratios to prevent undesirable hydrogen evolution.

This talk discusses the modelling of *in-situ* neutron reflectometry conducted on these reactive surfaces. The modelling of these data sets can be erroneously biased by restrictive and incorrectly deduced bounds especially when there is high uncertainty in the prior knowledge of surface morphology and composition. The method proposed here aims to avoid these pitfalls enabling automated modelling of the time-resolved data with data-led smoothing and evidence-based model selection.
Key points include:
• Automation for analysing large numbers of time-resolved datasets.
• Allowing the model to change between different time segments.
• Model selection using Bayes Factors.
• Smoothing infeasible outputs with data-driven bias.
• Dealing with multimodality in the posterior distribution.

Topics

Chemistry and Crystallography

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