NECEM SEMINAR: "Magnetic Resonance Studies of Solid-State Ionic Conductors"
Prof. Gillian R. Goward
From McMaster University, Canada
Tuesday 22nd October 2019, 2-3pm
Newcastle University, Room G36, Barbara Strang Teaching Centre (rear of Bedson bld)
Refreshments available after the seminar

Magnetic Resonance Studies of Solid-State Ionic Conductors
Prof. Gillian R. Goward, McMaster University, Hamilton ON, Canada

Understanding mechanisms and trends of Li mobility, diffusion, and aggregation in Lithium Ion Batteries (LIBs) is of paramount importance in order to characterize the properties of electrodes and electrolytes in functioning cells. Similarly, properties of proton-conducting solid-acids must be understood in order to properly utilize these materials in fuel cells (FCs). In both cases, the properties of the conducting ions can be specifically addressed using magnetic resonance imaging and spectroscopy.

This talk will give an overview of the applications of magnetic resonance techniques to such materials, using both ex situ studies of parent materials, as well as in situ studies on functional electrochemical cells. Our group have studied several Li+ and H+ conducting solid-state electrolyte and electrode materials, utilizing a range of magnetic-resonance strategies to compare and quantify ion transport processes. For example, 1H double quantum and exchange ssNMR reveals different exchange rates for pathways within the popular solid acid, rubidium di-hydrogen phosphate. Additionally, our newest work in solid-electrolytes, which relies on 7Li spectroscopy acquired at 20T magnetic field strength, paired with pulsed-field gradient diffusion measurements, acquired under ultra-high gradient strengths. These methods reveal both the number of local environments involved in exchange, and the diffusion timescales, as a function of temperature. These methods, appropriate for solid-state electrolytes, are compared with our earlier work on in situ studies of concentration gradients in solution-state electrodes, and within graphite electrodes.

Finally, newly developed *in situ* NMR technique that can monitor both the anode and cathode simultaneously has shown great promise for tracking the Li distribution in a full cell, as well as identifying reasons for capacity loss that are not readily available from bulk electrochemical analyses. This is achieved through a cell that is designed to perform under fast magic-angle spinning (MAS) conditions. The state of charge, metallic Li plating and SEI formation was captured for the first charge/discharge cycle of a full electrochemical cell ($LiCoO_2$/graphite). The spectral resolution has been enhanced to the extent that different chemical species that are usually overlapped in NMR analyses are distinctly identifiable.

Biography

Prof. Gillian Goward, an Associate Professor in the Department of Chemistry and Chemical Biology at McMaster University, is the lead investigator on a four-year, collaborative Automotive Partnership Canada (APC) initiative on lithium ion battery materials, which brings together researchers from both academic and industrial fields, to tackle the development of techniques for studying lithium ion cells under operating conditions. The objective of the Goward research group is to investigate ion dynamics in electrochemically-relevant materials using advanced solid-state nuclear magnetic resonance (NMR) methods. Her research results will have a significant impact on providing more efficient experimental means of quantifying dynamics, with measuring time savings of a factor of 100, and enabling analysis of much smaller samples, such as extracted battery electrodes. Dr. Goward has a second extensive body of work on the use of NMR to probe ion dynamics in hydrogen-bonded structures. These methods allow the detection of relative ion dynamics in novel structures targeted for high-temperature, low humidity fuel cell applications.

Location

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