Probing the Chemistry of Fuel Cells with ^{71}Ga NMR Spectroscopy

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Fast oxide ion conductors play a critical role as electrolytes in solid oxide fuel cells that generate electrical energy from green fuels. Anionic transport in materials is facilitated by structural defects, which are challenging to observe due to their local nature, and often take the form of an atom with a *vacancy* or an *interstitial* (*i.e.,* an atom with a range of possible coordination numbers). Nuclear magnetic resonance (NMR) is arguably one of the most powerful structural determination techniques for identifying such chemical environments. The key limiting factor of spectral resolution must be overcome – this is exacerbated for 73% of NMR-active nuclear spins in the Periodic Table, which are known as *quadrupolar nuclides* (nuclear spin > ½), many of which have very broad peaks or powder patterns.

In this work, we demonstrate that it is possible to detect ^{71}Ga NMR signals from gallium-containing electrolytes, due to the resolution made possible by the 36T Series Connected Hybrid (36T-SCH) NMR platform and an ultra-high field, fast magic-angle spinning (MAS) probe, both of which are uniquely implemented and built in-house at the MagLab. The complex ^{71}Ga powder pattern shape is very accurately reproduced by computations featuring a symmetry-adapted configurational ensemble, which comprehensively *model site disorder* and *capture the defect chemistry* of an important class of electrolyte materials. Additionally, for comparison, ^{71}Ga NMR spectra acquired on one of the strongest commercial magnetic fields available (23.5T) are of poorer resolution and incompatible with our atomic-scale understanding of the structural defects.

Our results highlight the importance of achieving spectral resolution using ultra-high field solid-state NMR – this aids in unlocking the Periodic Table of NMR and paves the way for new opportunities to interrogate advanced materials of increasing complexity.

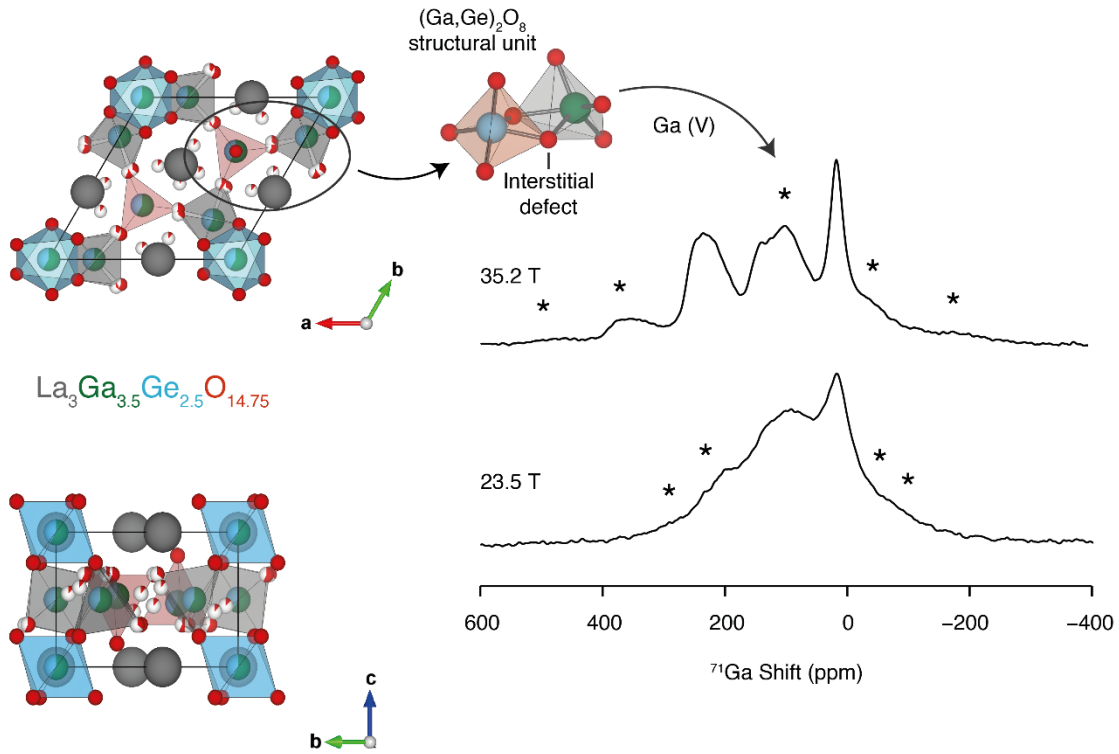

Figure *Left*: Defect chemistry of a gallium containing electrolyte (oxygens in red). ***Right*:** Resolved (35.2T) *vs.* unresolved (23.5T) ^{71}Ga solid-state NMR spectra and a disorder model. Asterisks (*) indicate artefacts (spinning sidebands).

Facilities and instrumentation used: Solid-State NMR Facility – 36T/40mm Series Connected Hybrid Magnet (35.2T/1.5GHz for ^{1}H NMR)

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