



High-Field NMR Study of Solid Oxide Fuel Cell

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

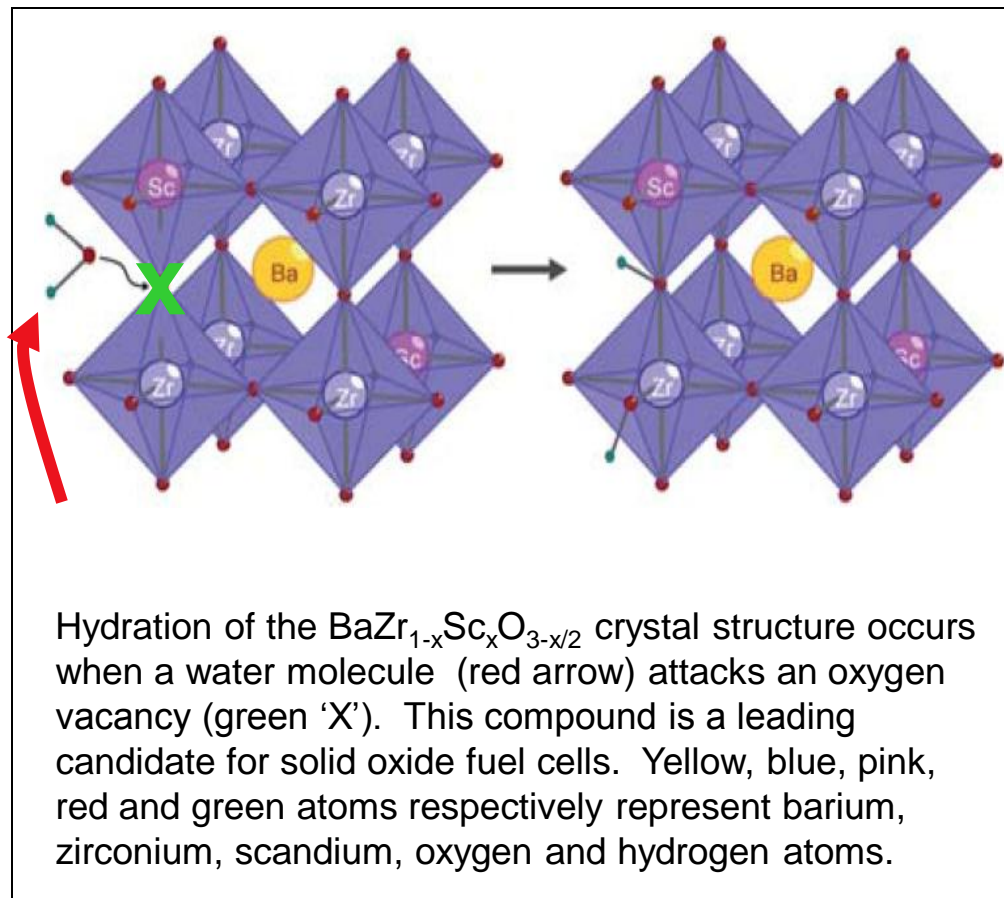
NMR User Program, FSU, Tallahassee



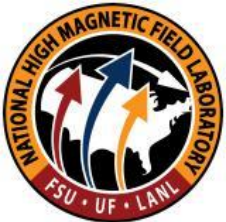
A Solid Oxide Fuel Cell (SOFC) is an electrochemical conversion device that produces electricity directly from oxidizing a fuel. Advantages of this class of fuel cells include high efficiency, long-term stability, fuel flexibility, low emissions, and relatively low cost.

The largest disadvantage is that the operating temperature is typically very high, resulting in long start-up times and problems with mechanical and chemical compatibility at elevated temperatures.

The Professor Clare Grey group at SUNY Stony Brook and Cambridge UK uses high field NMR to study protonic conduction pathways in scandium-substituted BaZrO_3 perovskite-type materials which show the best results as conductor in SOFC at lower operating temperatures.



This work supported in part by NSF/DMR-0804737, and the New York State Foundation for Science, Technology and Innovation via a NYSTAR award.



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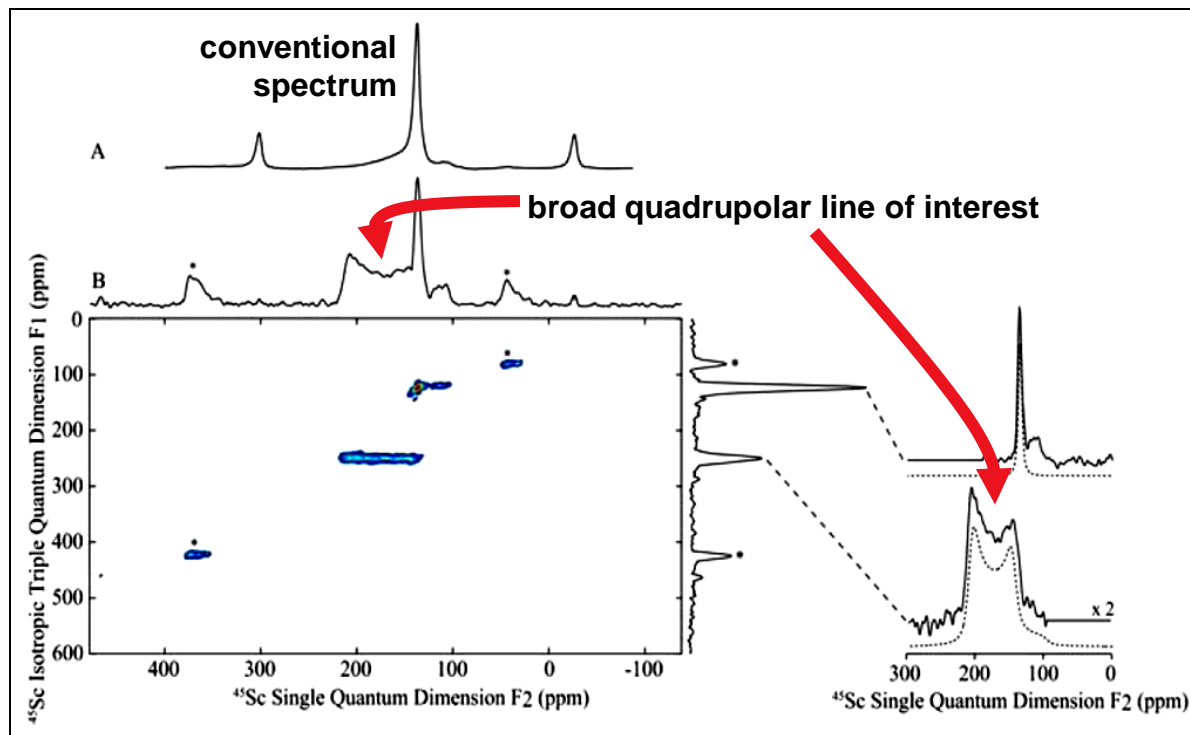
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- High-field (20T) NMR spectra taken at the NHMFL of scandium-substituted BaZrO_3 Scandium (^{45}Sc) multiple quantum magic-angle spinning (MQMAS) with Cq-selective spin-echo suppresses the bulk 6-coordinate Sc site, revealing the 5-coordinate Sc site associated with the oxygen vacancy responsible for the anionic conductance required for fuel cells to operate.



- The two-dimensional MQMAS resolves completely the broad and complex quadrupolar line shape (red arrows in figure) of the 5-coordinate Sc site for extracting electric-field-gradient and chemical shift parameters that are compared with quantum chemical calculations and known parameters to gain a detailed knowledge of the chemical processes in solid oxide fuel cells

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L. Buannic, F. Blanc, I. Hung, Z. Gan, C. Grey,
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