



NCCR MARVEL Distinguished Lecture

Structure and Dynamics in Batteries, Supercapacitors and Fuel Cell Materials: Application of New Experimental and Theoretical Approaches to Study Function

Prof. Clare P. Grey Department of Chemistry, University of Cambridge, Cambridge, UK

Wednesday 26th October, 17:15, Room MXF-1

Abstract: This talk will describe recent applications of NMR spectroscopy and pair distribution function (PDF) analysis of total scattering data to study electrode materials for energy storage and conversion. In particular, the focus will be on areas of our work where the combination of theory and experiment has been critical for interpreting experimental data and/or for understanding electronic structure. The use of ^{6,7}Li, ²³Na and more recently ¹⁷O NMR spectroscopy to investigate structural disorder, defects and dynamics in paramagnetic materials will be described. Examples include the development of methods to understand how Mg substitution in Na manganates affects rate performance of a series of layered phases in Na-ion batteries, to quantify stacking faults in intergrowth structures, and to investigate the transport mechanism in the ionic and electronic conductor La₂NiO₄₊. Many battery and supercapacitor materials are amorphous and methods to extract structure from these highly disordered systems and to determine the mechanisms for charge storage will be described.