NMR BEYOND LI: NA, MG AND LI-AIR BATTERIES

Tao Liu, Gunwoo Kim, Raphaele Clement, Phoebe Allan, Josh Stratford, Jeongjae Lee, Ieuan Seymour, Zigeng Liu, Clare P. Grey[§]

[a] *Chemistry Department, Lensfield Rd, Cambridge, CB2 1EW, UK*

cpg27@cam.ac.uk

This talk will describe the use of NMR spectroscopy to characterize a series of "beyond-Li" electrode materials. The NMR results are combined with complementary techniques such as pair distribution function analysis of (X-ray) scattering data. In the sodium-ion battery case, ^{23}Na NMR spectroscopy can be used to follow changes in local structure in a manner very similar to that performed on lithium-ion battery materials. Our work using the method to study local structure and Na^+ and electronic ordering in positive layered materials and intermetallic anodes will be described. ^{25}Mg NMR is more challenging, but the use of DFT calculations to predict shift positions and help interpret the spectra speeds up the analysis considerably. This will be illustrated for paramagnetic positive electrode materials. The use of NMR and MRI (magnetic resonance imaging) to link structural changes with electrolyte concentrations will be demonstrated for lithium metal anodes. Finally, new developments in the field of lithium-oxygen batteries will be described. In particular NMR spectroscopy allows the different discharge products and many side-reactions to be followed. For example, ^{1}H and ^{7}Li NMR spectroscopy can be used to separate Li_2O_2 from LiOH, allowing batteries that cycle via LiOH to be characterized. Our recent studies with LiI redox mediators and r-GO electrodes will be described.