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Towards a Net Zero World: Understanding Battery Function - New Metrologies, New Chemistries and New Insights

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More powerful, longer-lasting, faster-charging batteries – made from increasingly more sustainable resources and manufacturing processes – are required for low-carbon transport and stable electricity supplies in a "net zero" world. Rechargeable batteries are the most efficient way of storing renewable electricity; they are required for electrifying transport as well as for storing electricity on both micro and larger electricity grids when intermittent renewables cannot meet electricity demands. The first rechargeable lithium-ion batteries were developed for, and were integral to, the portable electronics revolution. The development of the much bigger batteries needed for transport and grid storage comes, however, with a very different set of challenges, which include cost, safety and sustainability. New technologies are being investigated, such as those involving reactions between Li and oxygen/sulfur, using sodium and magnesium ions instead of lithium, or involving the flow of materials in an out of the electrochemical cell (in redox flow batteries). Importantly, fundamental science is key to producing non-incremental advances and to develop new strategies for energy storage and conversion.

This talk will focus on our own work to develop NMR, MRI and new optical methods that allow electrochemical devices to be probed while they are operating, from the local, to particle and then cell level. This allows transformations of the various cell materials to be followed under realistic conditions without having to disassemble and take apart the cell. A good example is our work on $LiCoO_2$, where via optical approaches we were able to directly visualize movement of phase fronts as lithium is removed and inserted into this material. A strong focus of our work has also been on developing methods to link theory with experimental observations. For example, I will illustrate how a combination of NMR to measure transport (Li^+ hopping), X-ray diffraction (XRD) to measure phase segregation within the bulk, optical measurements to explore processes at the particle level, and continuum modeling to tie transport with particle level observations, can be used to study electrode material function, focusing on Ni-rich NMC cathodes. Recent results exploring graphite flakes and faceted single crystal particles and interparticle interactions via optical experiments and theory will be described. In the final part, I will explore intercalation mechanisms and degradation modes in lithium-nickel oxide cathodes, connecting experiment (^7Li hyperfine shifts and XRD) with density functional theory calculations of local structure, Jahn Teller distortions and dynamics. New results on extremely high-rate batteries will be outlined; I will then illustrate how our new metrologies can be extended to study a wider range of electrochemical systems.