Salt Effects on Li-ion Exchange Kinetics and Activation Energies – Systematic In Situ Synchrotron Diffraction Studies

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Solid state ionic conduction plays a central role in the functionality of many energy materials, including the cathodes being used in the present generation of battery technologies and the solid state electrolytes being considered for the next generation of batteries. Solid state ion exchange of Li+ into Na2Mg2P3O9N was investigated using in situ synchrotron powder X-ray diffraction. By using a 2D area detector many samples were studied simultaneously in novel high throughput studies of ion exchange reactions. Kinetic rate constants were extracted from the time-dependent evolution of lattice parameters. Reactions were followed using a novel on-the-fly Rietveld refinement tool which enabled real time monitoring of reaction progress. The ion exchange rates were found to be limited by the ion transport in the salt rather than the host ceramic. From this data, it was seen that reaction rates substantially varied with salt concentration in a manner than appears to follow a universal scaling relationship. By carrying out experiments at different temperatures, activation energies for reactions could be precisely determined. The origin of the experimentally observed activation energies is being investigated through DFT studies.