Probing ion mobility in lithium- and sodium-ion conductors for a clean energy future

Battery development is a pertinent research topic as the sustainable industry continues to grow. At the current state, we have means of obtaining enough renewable energy such as solar, wind, etc. but the storing and distribution of this energy across the globe has proven to be an incredible challenge. Current batteries employ liquid electrolytes that conduct ions, but pose many serious problems, including safety, thermal runaway and are toxicity. To circumvent these challenges, solid ionic conductors, known as solid state electrolytes (SSEs) are being developed which promise greater safety and either equivalent or better performance.[1] Although lithium-ion batteries are the current market leader, the high abundance and size of sodium makes it more cost and energy effective, particularly for large-grid storage systems. Albeit, these have to meet certain strict requirements before they can be used in batteries commercially, including high volumetric energy and power densities, low electronic conductivity, and efficient rechargeability. The process of developing SSBs involves the development of SSE, the cathode and the anode.

My research project will seek to evaluate how slight changes in the structure of the solid state electrolyte and cathode can can impact the ionic conductivity of lithium and sodium-ion batteries. Along with the structure, focusing on the surface of the SEs is very important: high bulk conductivity of SSEs results in a high ion migration barrier between the electrolytes and the electrode, resulting in electrolyte-electrode interface impedance being a key fabrication point with batteries. LISICON (Lithium Superionic Conductors) were first synthesised as possible ion conductors and different compositional doping strategies were tested and evaluated for their effects. Li ions occupy interstitial holes in LISICON. Dopants such as Al, Ge, As helped increase the number of interstitials hence altering the Li diffusion mechanism from local oscillations to superionic flow. Multi-dopant strategies such as the Ta doping over the Al dopant structure increases the space for Li-ion transport by changing energy favouring sites. [2-3] DFT and computational calculations will be employed to detect which crystallographic sites are available and how the mechanism of 3D Li-ion movement will change.

Incorporating this research into the development of NASICONs (Sodium Superionic Conductors) proves to be a slight issue due to the large mismatch in ionic radii between the sodium and lithium ions and greater covalent character of Li-O compared to Na-O bonds. [4-5] Alterations to ensure maximum compatibility have been made with the electrode and electrolyte will be investigated using spectroscopic techniques such as variable temperature NMR spectroscopy. An in-situ cell will be used to trial different electrolyte-electrode combinations to determine their conductivities, with the cell being electrochemically cycled at the same time as investigated molecular level changes via NMR spectroscopy, specifically exploring ion mobility.

Contact will be made with automobile companies like NationalGrid, Nyobolt, Aquion Energy and some startup companies in the final weeks of the first summer to secure a placement for the second year. I will specifically seek to work in the research-to-commercialisation part of these companies, as my main interest is how the current research findings are being implemented into manufacturing large energy storage systems. In light of COVID-19, arrangements such as online calls and learning may need to be conducted, but this will not impact my knowledge as I will endeavour to apply industry knowledge on a smaller scale into further hands-on lab experience at my university.

Around the world, global, national, local scales require different amount of energies. Working at a smaller scale rather than a large one (e.g. national grid storage) with my minimal research would be more feasible. Thus, it would be best to work with equipment such as AED (Automated External Defibrillators) [6] which delivers high current pulses and requires the storage of large amount of energies. For my Leadership in Action project, I would like to design, lead and produce a small-scaled prototype sodium battery based on the most compatible electrolyte-electrode materials and put that to test on current equipment. Differences and similarities in the energy output between the prototype and existing batteries will be observed and studied. Whilst I currently believe working at this scale would be the most appropriate approach for the second summer, receiving offers from certain companies I share very similar ethos and values will mean I will be likely to change my planned approach.