Final Report

Project acronym: *NEILLSBAT*
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Publishable project summary

The project developed novel approaches for batteries for stationary storage through the development of high-capacity anodes based on silicon and silicon/germanium nanowire heterostructure arrays in addition to safe non-flammable ionic liquid electrolytes. Briefly, silicon as an anode material in a lithium battery undergoes a different lithiation mechanism to graphite which is the most commercially used anode. This mechanism is an alloying process where Si alloys with Li in first cycle to produce Li4.4Si allowing very high storage capacity. A disadvantage with alloying is the resultant volume expansion that occurs which with typical particle sizes used for active material (tens of microns) reults in shattering of the particles. The UL approach is to develop this material in nanowire form directly with growth occurring directly from the electrode substrate. This eliminates binders and conductive additives and increases the overall energy density of the battery. A major issue in rechargeable batteries also is the low flash point of the solvents used as electrolytes with significant safety implications. The transition from organic electrolytes to ionic electrolytes provides for a much more safe battery chemistry for commercial application. Iolitec developed F-free ionic liquids (ILs) and Li salts as potential electrolyte components for example N-propyl-N-methylpyrrolidinium dicyanamide. Experiments were also carried out on metal organic frameworks which are porous materials consisting of architectures of nodes and linkers with the aim of using these as host for S in LiS chemistries with ionic liquids. A range of MOFs and MOMs were studied with the observation that the porous frameworks were unstable in the presence of electrolytes rendering them unsuitable for application in full cell batteries versus silicon anodes. In works by UL and KIT we did observe that the MOFs could be converted by anneal into active electrode materials for lithium ion. The optimal full cells prepared by KIT included a LiFePO4 cathode against the Si NW anode achieving an energy density (< 500 Wh kg-1, based on the active materials weight), with the silicon nanowires combined with ionic liquids which is one of the few examples of a fully F-free battery and could be considered as a viable and environmentally friendly system for stationary storage. In this project, under Topic 4 Functional Materials section 4 Energy Storage, we were able both to synthesise these high performance electrode materials and also achieve a detailed understanding of their structural and chemical evolution during battery cycling.