Integrated Computational and Experimental Study of Sodium Intercalation Cathode Materials

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Developing cheap, environmentally friendly energy storage solutions are necessary to accelerate the adoption of renewable energies and to reduce carbon footprint. Conventionally, over the past few decades battery technology research has mostly focused on Li ion based technologies predominantly due to its high gravimetric and volumetric capacity. However, the recent adaptation of large scale smart grid technologies has necessitated the need to cheap, safe and environmentally friendly battery technologies. Sodium ion based battery technologies can help solve these challenges, since sodium, compared to Lithium is an earth abundant and safe metal. Developing Na batteries require development of high voltage, capacity cathode materials. In this work, we employ integrated computational and experimental approaches to systematically study two different families of cathode materials namely (i) sodium manganese oxide[1] and (ii) alludite type sulphate based[2] materials. We systematically explore how modifying materials chemistry influences their electrochemical properties. Further, we also explore how the change in Na stoichiometry influences material structure, ion transport and electron transfer characteristics of the materials that are critical in determining the cathode performance. We employ the knowledge gained from this material to optimize the material structure and chemistry. Further, we also transfer information obtained from atomistic scale studies to mesoscale systems that can lead to identification of the best electrode/electrolyte combination that can provide the best battery performance.

References:

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