Thesis title:

Molybdenum Disulfide Based Composites for Sodium-ion Batteries

ABSTRACT

Over the last many decades, lithium-ion batteries (LIBs) have dominated the market of portable electronics, electric vehicles and grid-scale energy storage. There is a growing demand for alternative battery chemistries, which can address key challenges and limitations posed by LIBs, both in terms of cost and geopolitical issues. Sodium-ion batteries (SIBs) have attracted significant attention as a viable alternative to advanced LIBs. This shift in focus is primarily attributed to the abundance of sodium resources and easy access to associated knowledge of electrochemistry in SIBs, which is similar to LIBs. Sodium is the fourth most abundant material in the earth's crust and its resources are widely distributed throughout the globe. Consequently, the cost of sodium as a source material is substantially lower compared to that of lithium.

However, SIBs face significant challenges due to the substantially larger ionic size of Na^+ compared to Li^+. With an ionic radius of approximately 1.02 Å, Na^+ are about 34% larger than Li^+, which have an ionic radius of about 0.76 Å. As sodium-ions intercalate into and de-intercalate from the electrodes, they induce more pronounced expansion and contraction of the crystal lattice. This leads to increased mechanical stress, which ultimately leads to structural degradation over repeated charge-discharge cycles. Consequently, the electrode's stability, cycle life and the overall performance of SIBs is compromised. Hence, to promote SIBs as a viable alternative, fabrication of high-performing and stable anode materials is essential. Molybdenum disulfide (MoS_2) is an inorganic compound belonging to the transition metal dichalcogenides (TMDs) family. It has one atom of molybdenum sandwiched between two atoms of sulfur. Exfoliated MoS_2 can serve as a suitable candidate for next-generation SIBs, owing to its layered characteristics. However, comparatively poor electronic conductivity and high-volume expansion hinders its large-scale usage. Therefore, during this work, several steps were taken to overcome these limitations.

In this thesis, it has been established that optimization of exfoliation time is critical to extract best performance in such layered materials. MoS_2 was exfoliated using liquid phase exfoliation (LPE) method, for varying duration. Physiochemical and electrochemical tests were subsequently performed to assess the Na-ion storage capabilities of the exfoliated MoS_2. To further improve the performance, nitrogen-doped carbon MoS_2_NDC composites were synthesized and evaluated. These demonstrated exceptional capacity and stability as anodes for SIBs. Using the optimized anode and cathode materials, full cells of SIBs were fabricated and characterized. The performance of these batteries is also discussed in the work. For the full cell fabrication, MoS_2_NDC anode was used along with NFP as the cathode material. Ex-situ analysis after hundred charge-discharge cycles provided insight into the cell's performance, confirming its feasibility in real-world applications. Using LCA studies, it is also shown that the fabricated SIBs have much lower carbon footprint than commercially available LIBs.