Summary

The promotion of climate-aware and environmentally friendly sustainable energy technologies necessiates an increasing demand for mobile energy storage devices. Lithium ion batteries (LIBs) have a very pronounced energy density (100-265 Wh/ kg), and they are the materials of future when it comes to the efficient energy storage during utilization of renewable energy technologies such as solar energy and wind energy. In order to achieve the visions related to the accelerated design and discovery of ultra-high performance batteries, it is necessary to guarantee the performance-reliability synergy in this category of energy storage materials. Dendrite formation at anode and growth is an interfacial process spanning numerous length- and time scales; and regardless of decades of research, their composition, structure and formation still present a significant conundrum. Lithium dendrites are responsible for problems like short circuits, catastrophic failures and fires, electrolyte decomposition, and loss of active lithium in the battery. The achievement of completely dendrite-free battery interfaces can be possible only through the correct understanding of the fundamental mechanisms governing the dendritic evolution. This research proposal titled as "**Learning the Physics of Dendrite Growth in Lithium-Ion Batteries: An Attention Mechanism Approach for Prevention and Mitigation (Acronym: DENDRITEPHASE)**", presents the multifaceted approaches in linking the microstructure-property and process-kinetics relationship in the different material phases of an electrochemical battery through integrated experiments, computations and artificial intelligence, to subsequently demystify the dendrite evolution mechanisms. For the variants of LIBs printed using fused deposition modeling, the geometry and morphological feature information will be monitored through experiments. This time-dependent spatial information about the phase microstructures of the interface will be then relayed to the finite element analysis. The atomistic simulations informed phase field model will be able to distinguish the roles of anisotropy, intermediate phase reaction kinetics, ion transport and mechanical loading in deciding the fate of dendrite structure. In order to expedite the determination of material properties for use in the phase field model, graph attention network will complement the density functional theory (DFT) and molecular dynamics calculations. The computational datasets on structure, properties and behavior of battery materials, combined with the experimental datasets of temperature, voltage and other physical quantities will be employed to construct attentive generative AI models. The microstructure reconstruction through the variational autoencoders (VAE), will be used for discovering the electrode and/or electrolyte materials exhibiting anomalous behaviors in relation to dendrite nucleation at solid electrolyte interface (SEI). The VAE will be integrated with gaussian process regression to locate optimal nuclei sites at SEI that correspond to dendrite suppression. Two types of transformer models - composition generators and structure generators, will be utilized to design and discover new battery materials that reveal dendrite inhibition characteristics. The interlinking among all the modules ensures that the diverse features from DFT (e.g. adsorption energy, formation energy, interface energy, elastic moduli), experiment (overpotential, porosity of supportive structure at anode), and finite element analysis (order parameter corresponding to electrode , elastic deformation of solid electrolyte) will be standardized into a common pool of physically intuitive features before using in the attention mechanism based VAE and transformers.