| Berkley: | BOYU QIE | Energy devices

| Cambridge: | May Ching LAI | Electron Microscopy of energy materials

# Research Proposal: Investigating the Nanoscale Properties of Cathode Materials and Their Potential Applications in Energy Devices

## Objective:

The objective of this research proposal is to combine the research efforts of May Ching Lai and Boyu Qie to investigate the nanoscale properties of cathode materials for lithium-ion batteries and explore their potential applications in energy devices.

## Introduction:

The rapid advancement of cathode materials for lithium-ion batteries has been driven by the need for high-capacity, long cycle-life, and superior safety in energy storage systems. Li(Ni0.8Mn0.1Co0.1)O2 is considered as one of the most promising cathodes; however, issues such as particle cracking are thought to limit its structural stability and long-term cycling performance. Understanding the properties of cathode materials at the nanoscale is crucial for advancing electric vehicles.

## Methodology:

To achieve the research objective, a combination of electron microscopy techniques will be employed. Battery cells will be synthesized and electrochemically cycled by collaborators, producing samples for analysis. May Ching Lai will utilize focused ion beam-scanning electron microscopy (FIB-SEM) to prepare thin lamellae for transmission electron microscopy (TEM) studies. FIB-SEM tomography will be performed, and 3-dimensional models will be created using Dragonfly software. TEM techniques, such as energy dispersive X-ray and electron energy loss spectroscopy analysis, will evaluate the distribution of transition metals. Additionally, diffraction patterns and high-resolution TEM will provide information on crystal structure, strain, and cracking. The data obtained from TEM will be analyzed using the Hyperspy Python library for multidimensional data analysis.

Boyu Qie's expertise in energy devices will be utilized to explore the potential applications of the cathode materials. Wet lab synthesis and on-surface synthesis techniques will be employed to fabricate novel energy devices. Scanning probe microscopy will be utilized to characterize and image the fabricated devices. Additionally, device fabrication and electrochemistry experiments will be conducted to evaluate the performance of the energy devices. Quantum chemistry simulation, periodic system simulation, condensed matter theory, and machine learning and AI techniques will be employed to further understand the complex materials and optimize the energy device performance.

## Expected Outcomes:

The combined research efforts of May Ching Lai and Boyu Qie will provide valuable insights into the nanoscale properties of cathode materials, contributing to the understanding of their structural stability and long-term cycling performance. Moreover, this research will explore the potential applications of these materials in energy devices, furthering the development of clean energy and energy-efficient technologies.

## Keywords:

Electron microscopy, focused ion beam, scanning electron microscopy, energy dispersive X-rays, electron energy loss spectroscopy, wet lab synthesis, on-surface synthesis, scanning probe microscopy, device fabrication, quantum chemistry simulation, periodic system simulation, condensed matter theory, machine learning, AI, electrochemistry.