THE PHYSICS OF HOW MATERIALS STORE ENERGY

Hillary Smith
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How does the structure of the battery change at the atomic level when lithium is inserted into and extracted from the cathode of a lithium-ion battery?

What changes occur in local electron dynamics when the battery is charged and discharged?

What is the thermal stability of materials for storing hydrogen relate, and how does this relate its adsorptive properties?

Does the specific heat capacity reveal any thermal behavior that can suggest ways to optimize the adsorption process?
Why Do We Care About Energy Storage?

Energy storage is important for stationary power, portable power, and transportation.

Global Access to Clean Energy

The development of higher-capacity battery cathodes will not only enable cheaper portable electronic devices, but can be used in combination with solar cells to store energy in parts of the world without connection to the energy grid.

Sustainability

Understanding how secondary battery systems in hybrid vehicles degrade over time could allow them to be recycled in stationary energy storage applications after they are no longer of use in the vehicle.

Materials are crucial to the development of socially-responsible alternative energy solutions.
My research makes connections between a material’s [thermodynamic, magnetic, structural] properties and its utility for a functional application [like in a battery]
Polaron Mobility and Disordering of the Sodium Sublattice in Triphylite-Na$_x$FePO$_4$

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Supporting Information

ABSTRACT: The interplay between sodium ordering and electron mobility in Na$_x$FePO$_4$ was investigated using a combination of synchrotron X-ray diffraction and Mössbauer spectrometry. Synchrotron X-ray diffraction measurements were carried out for a range of temperatures between 298 and 553 K. Rietveld analysis of the diffraction patterns was used to determine the temperature of sodium redistribution on the lattice. This diffraction analysis also gives new information about the phase stability of the system. Mössbauer spectra were collected in the same temperature range. An analysis of the temperature evolution of the spectral shapes was used to identify the onset of fast electron hopping and determine the polaron hopping rate. The temperature evolution of the iron site occupancies from the Mössbauer measurements, combined with the synchrotron diffraction results, shows a relationship between the onset of fast electron dynamics and the loss of local order on the sodium sublattice.
EXPERIMENT AT OAK RIDGE NATIONAL LAB
SUMMER PROJECT I

Thermal Analysis and Heat Capacity Study of Cathode Materials for Na-ion Batteries

- What is the thermal stability of materials for sodium batteries, and how does this relate to its electrochemical properties?
- Does the specific heat capacity reveal any thermal behavior that can suggest ways to improve the battery?

SUMMER PROJECT II

Investigation of Olivine NaFePO$_4$ and Mixed-Metal Fluorides with Diffraction and Mossbauer Spectroscopy

- How does the structure of the battery change when lithium is inserted into and extracted from the cathode of a lithium-ion battery?
- What changes occur in local electron dynamics when the battery is charged and discharged?
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<th>SUMMER PROJECT I</th>
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<td><strong>THERMAL PROPERTIES OF BATTERY MATERIALS</strong></td>
<td><strong>STRUCTURE/PROPERTY RELATIONSHIPS IN SODIUM ION BATTERY MATERIALS</strong></td>
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<tr>
<td>• Preparing new materials for characterization</td>
<td>• Calibrating and using our new Mossbauer spectrometer</td>
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<td>• Measuring heat capacity using our new calorimetry system</td>
<td>• Performing electrochemical cycling of batteries</td>
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<td>• Characterizing materials with x-ray diffraction</td>
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<td>• Analyzing data collected at the SNS (Spallation Neutron Source at Oak Ridge National Lab) on the structure as function of temperature</td>
<td>• Analyzing data collected at ANSTO (Australian Nuclear Science and Technology Organisation) of the structure of the battery during operation</td>
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WHAT YOUR SUMMER WOULD LOOK LIKE

• working with new equipment and tools in the lab
• making samples and testing them
• analyzing data with Igor and Python

Beyond Summer 2020

• Possibility for semester or thesis work
• Possibility to travel to a national lab for experiments
• Possibility to present results at a national meeting/conference

I’M ALWAYS HAPPY TO TALK ABOUT THESE EXCITING TOPICS!
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