High-entropy Oxides With Lithium Batteries

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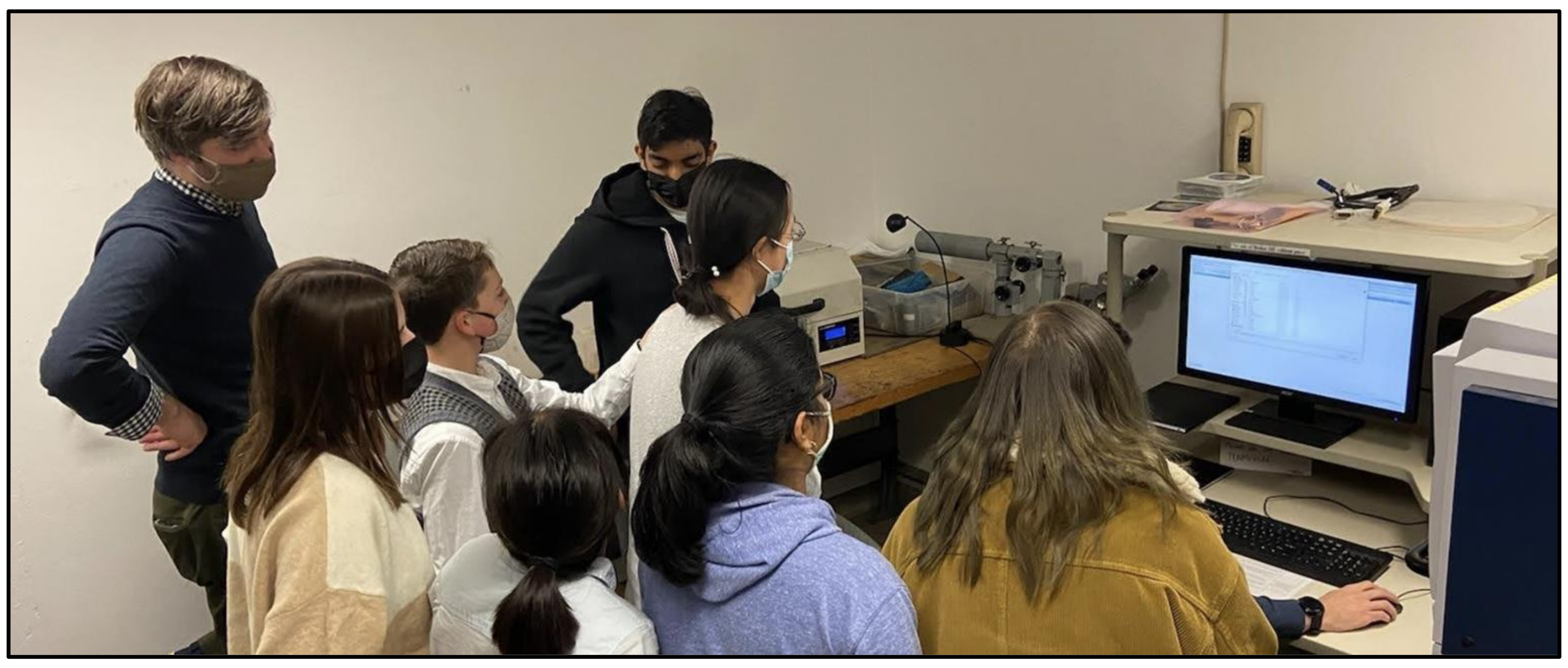
Motivation

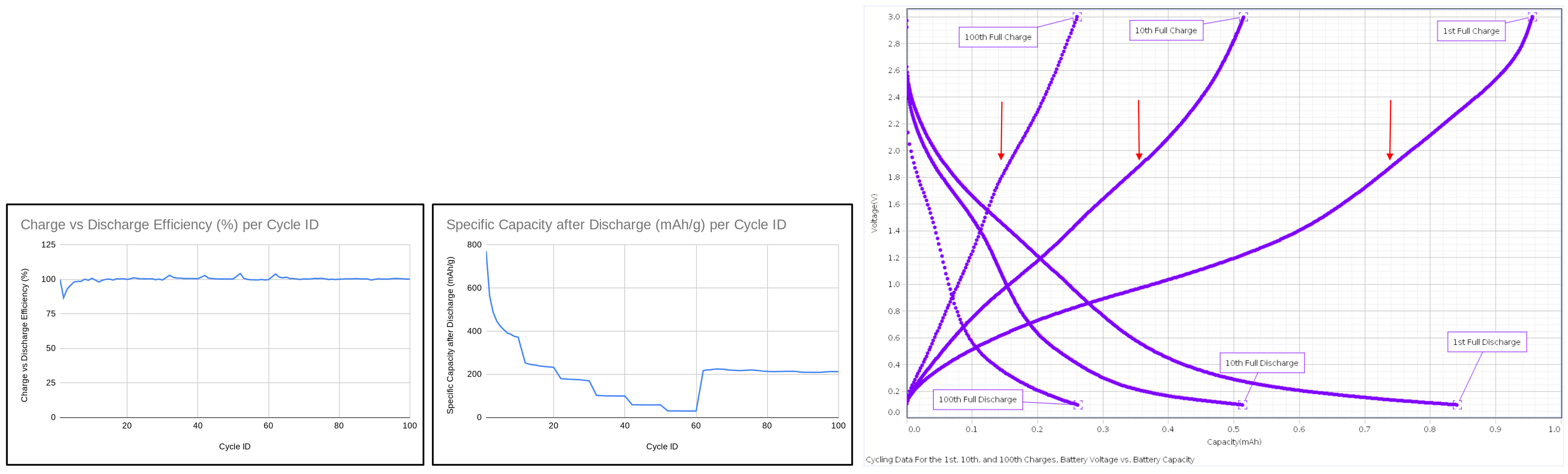
- A growing preference for green, non-carbon-dependent energy sources has led to heightened demand for reusable energy.
- We are looking to research a new compound that can be used in a lithium-ion battery (LIB) in order to maximize voltage, current, and cycle integrity.
- We are exploring the emerging field of High-entropy Oxides (HEO), an oxide which includes 5 or more metal cations.
- This will increase the configurational entropy of the oxide, allowing the lithium ions to pass through the structure via multiple paths.
- We will specifically be investigating the oxide $(V_{0.2}Cr_{0.2}Nb_{0.2}Mo_{0.2}W_{0.2})O_x$



Major accomplishments

Battery Cycling Data

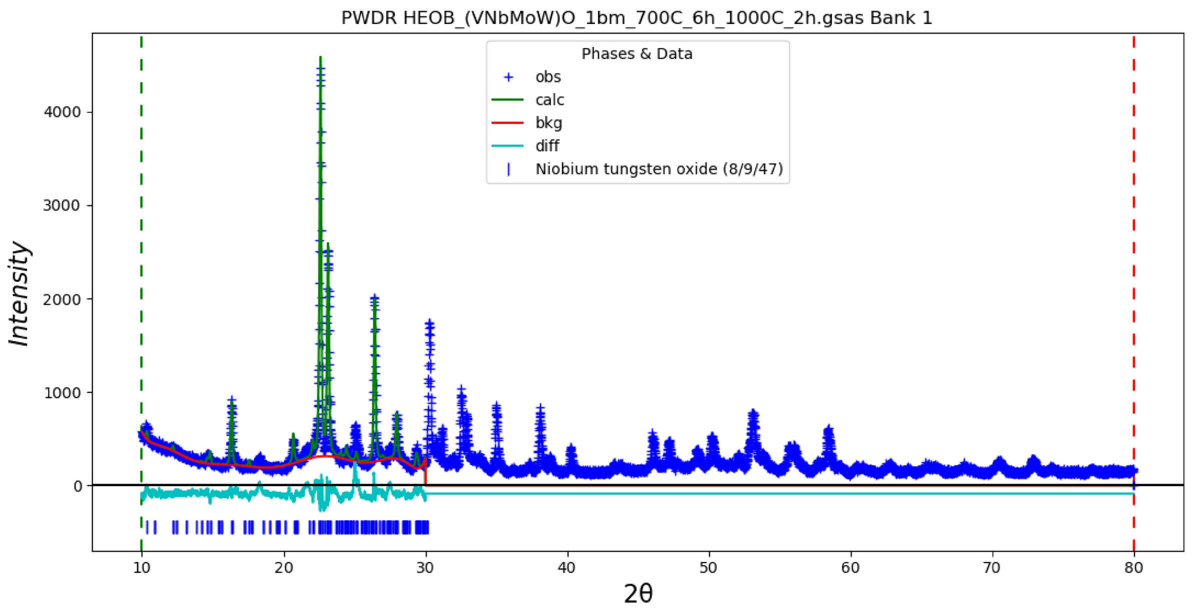
- The charge/discharge efficiency of our cell remained at or very near 100% over 100 cycles
- As seen in the graph below and to the right, the capacity of the cell decreased until around the 60th cycle, at which point it maintained a stable capacity
- Despite the decrease in capacity, the voltage at which the redox reaction occurs in the cell remains constant. This is shown in the graph below with red arrows indicating the small bumps in the voltage vs. capacity curve, all of which occur at approximately 1.9 V.



The battery cycling data shows how the battery efficiency stabilizes at 100% after 60 cycles. This indicates that the battery could still efficiently hold a charge.

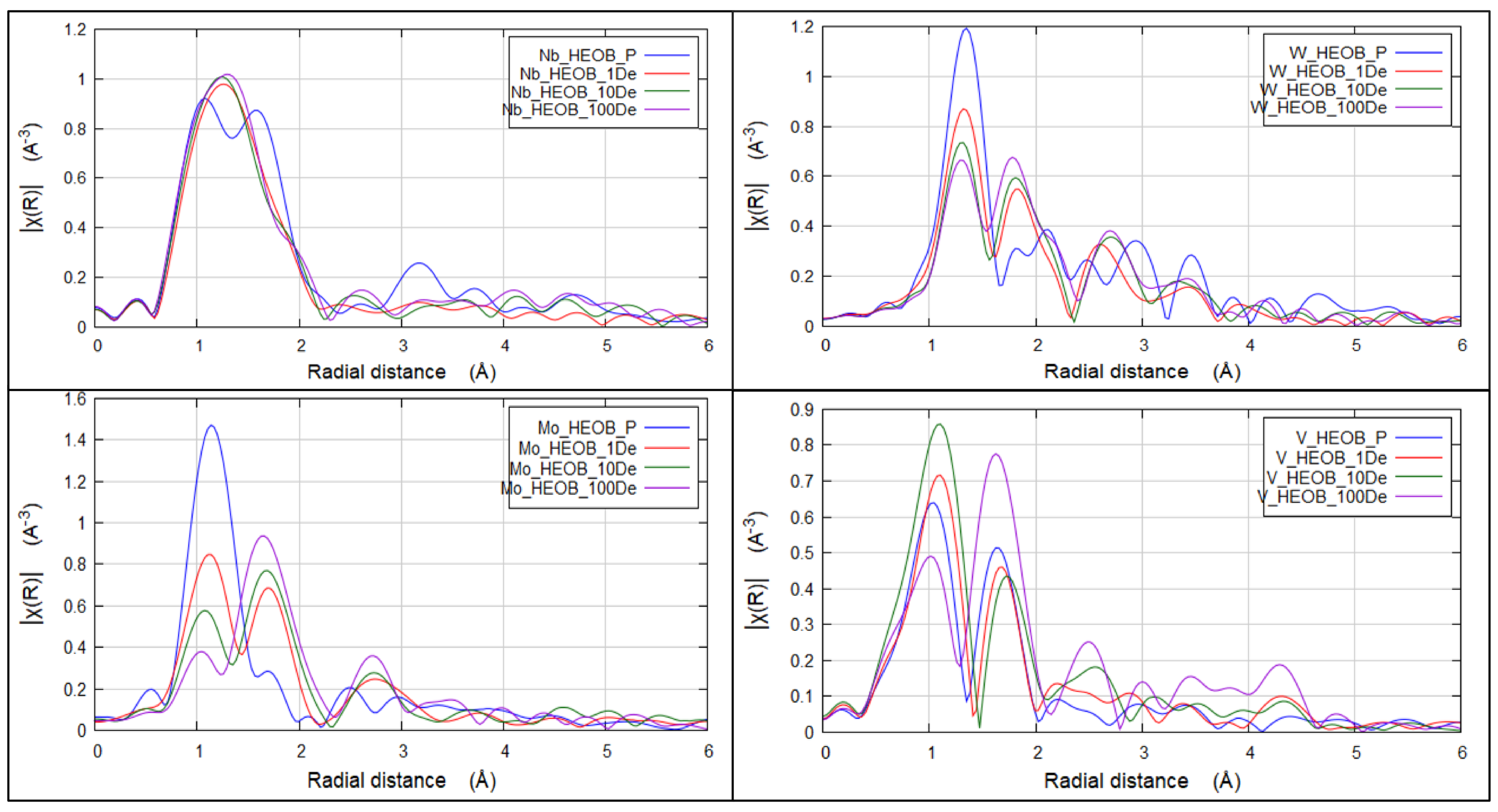
X-Ray Diffraction Data

- X-ray Diffraction shows the structure of the crystalline structure. Peaks from the analysis can help us understand the lattice structure and gives an insight into the distribution of atoms in a lattice plane



Extended X-Ray Absorption Fine Structure (EXAFS) Data

- For each element, there is a tendency for the first peak to drop and the second to rise with cycling, signaling that there's a loss of shorter bond lengths and a change in the valence. This shorter bond length is not recovered
- The elements continue to oxidize during the structural changes and never turn into metals
- By 100 cycles, each transition metal reaches a steady-state where there isn't a large change in valence or structural parameters as a function of cycling, showing a stable structure is reached



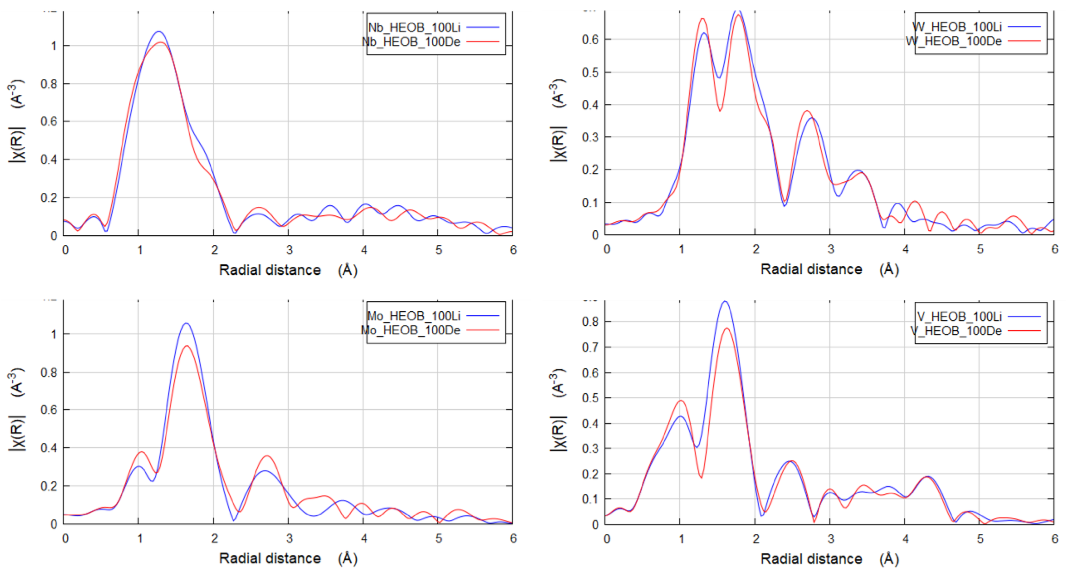
Battery cycling data shows the different delitiation states and the magnitude of oxidation over radial distance.

Conclusion

- Three different cells maintained, after 100 cycles, a charge-discharge efficiency of around 100%, suggesting that the battery is viable
- The absorption edge for all constituent elements did not deviate significantly from its initial edge
- Similar results were obtained by researchers at the University of Cambridge, who documented that the tungsten niobium oxide anode can possess many lithium diffusion channels within its structure, leading to a remarkably high discharge rate
- The atomic structure we simulated in Vesta supported our hypothesis, showing an incredibly large lattice parameter of 36 Å as well as a wide-open structure that, as proven by our battery cycling data, allows for extremely fast and efficient charging and discharging

Future Direction

- The cell was left exposed to the atmosphere while waiting to be measured, and we believe it self-oxidized because there was a minimal amount of change in the local structure between the lithiated and delithiated state (EXAFS). Therefore, we cannot determine if there are structural changes during lithiation, given the current EXAFS data.
- In future research we recommend a repeated experiment to accurately gage the structural changes during the lithiation and delithiation cycles.
- We suggest performing in situ measurements of the lithiated anode to get a better picture of how the battery changes before and after lithiation.



Evidence of self-oxidation is most notable between the 100th delithiated and 100th lithiated states of each element

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