

NICKEL SULFOSELENIDE ELECTROCATALYSTS FOR FLOWING ZINC-AIR BATTERIES

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Background

Project Goal

Study nickel mixed chalcogenides electrocatalysts to enable **rechargeable** Zn-air batteries to determine **what** S/Se mixture provides the best performance and **why**.

Current Practice

Zn-air batteries are **non-rechargeable low-current cells**, or else rely on expensive electrocatalysts for recharge. Batteries limited to **single-use** or **cost prohibitive** to build at scale.

Why SNL?:

Sandia has institutional knowledge of Zn-based batteries and researchers with extensive experience bridging electrocatalyst materials and battery research.

Innovation

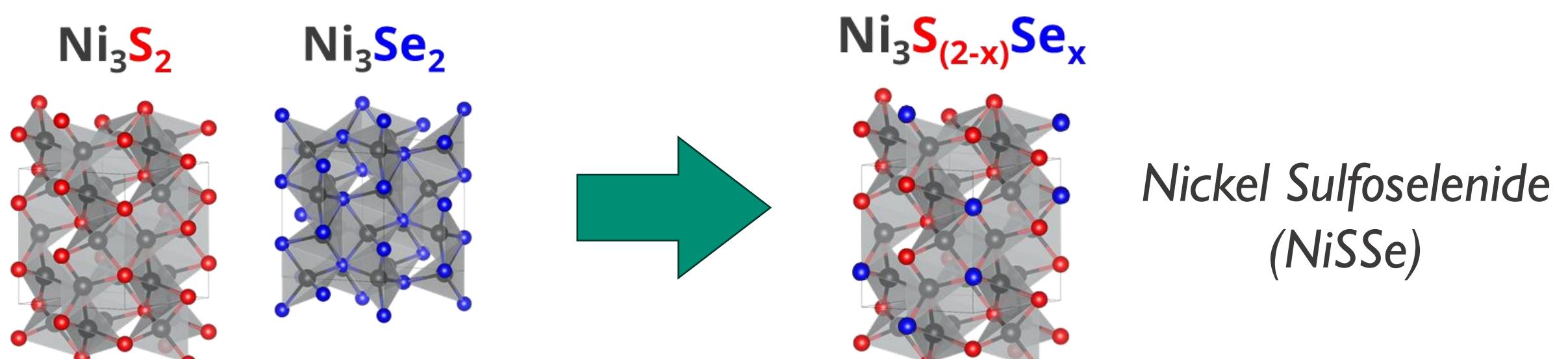
We are exploring hitherto **understudied metal sulfoselenides** as electrocatalysts alongside the use of flow cell architecture to improve battery performance.

Impact

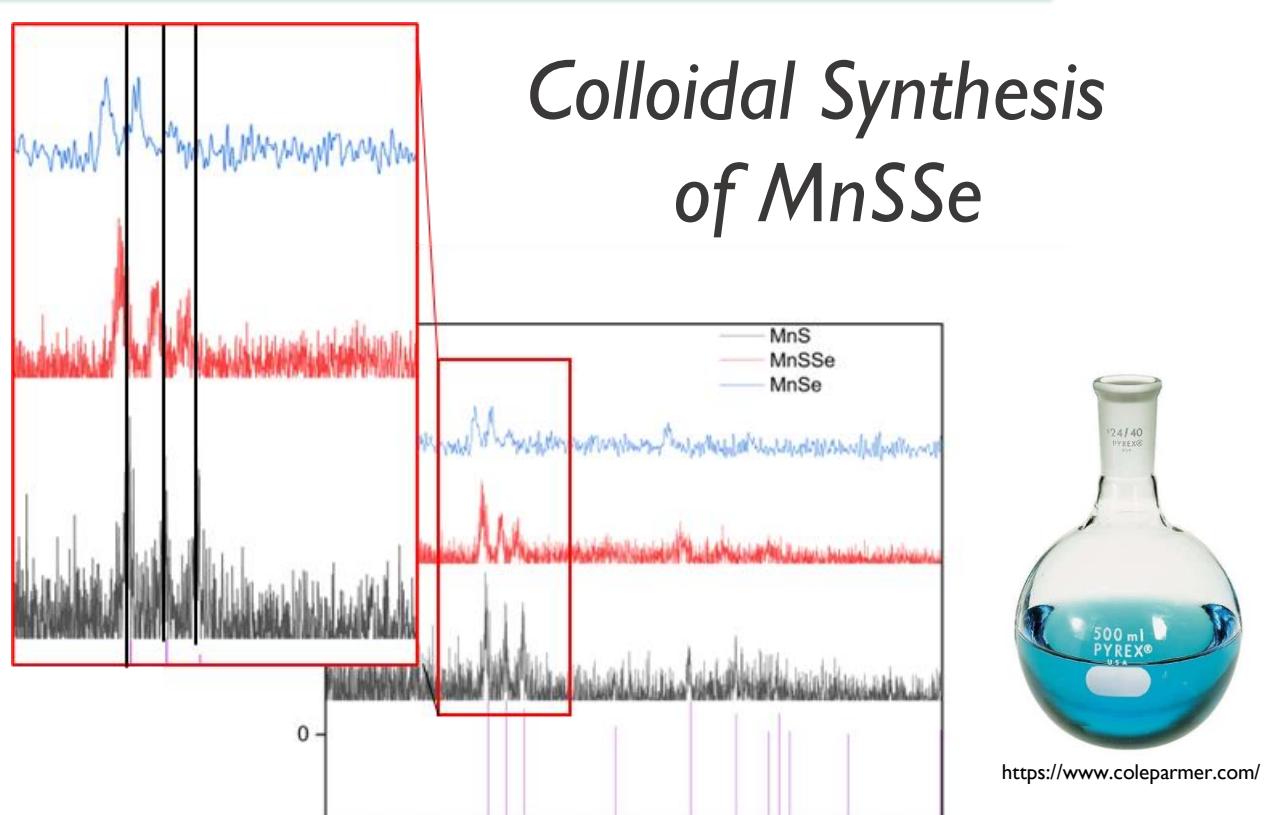
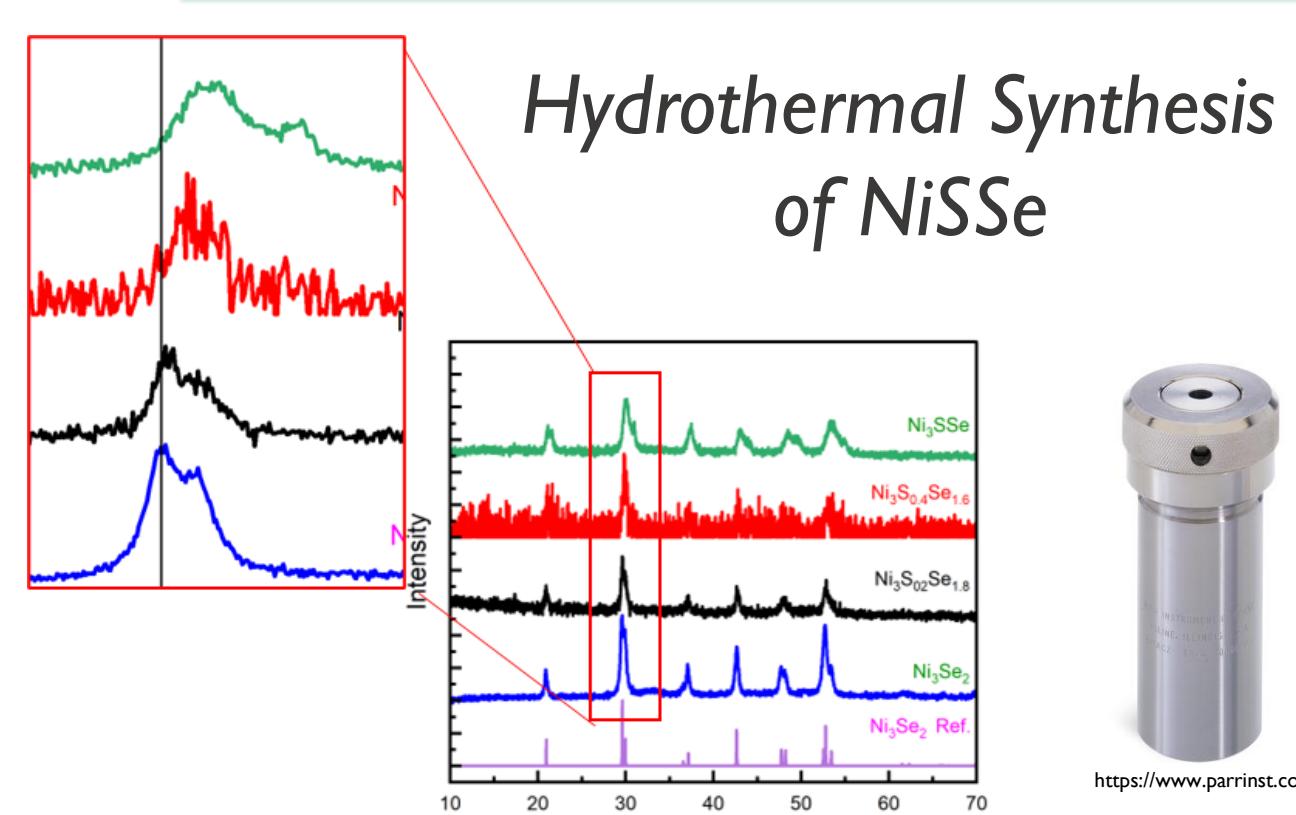
Battery startups working on Zn-air batteries would benefit from **precious metal-free electrocatalysts**. New electrocatalysts have broad use in many **energy storage and production technologies** (batteries, fuel cells, electrolyzers).

Alignment

Zn-air batteries use earth-abundant metals (**affordable, secure**) to **reliably** deliver electricity, while bolstering American scientific innovation and improving supply chain security (*Unleash American Energy Innovation*) to provide **reliable and safe energy generation** for the US electrical grid (*Strengthen Grid Reliability and Security*).

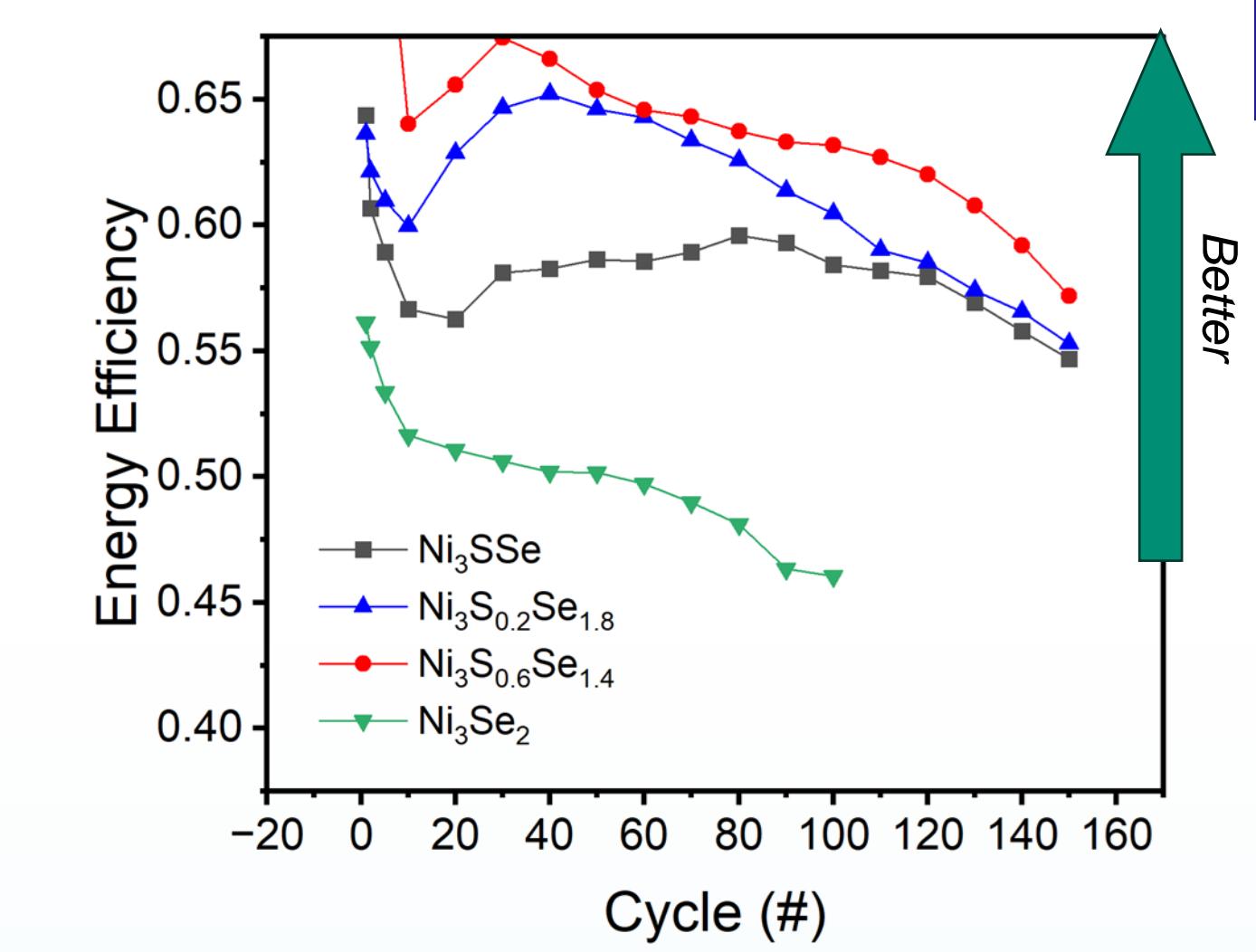
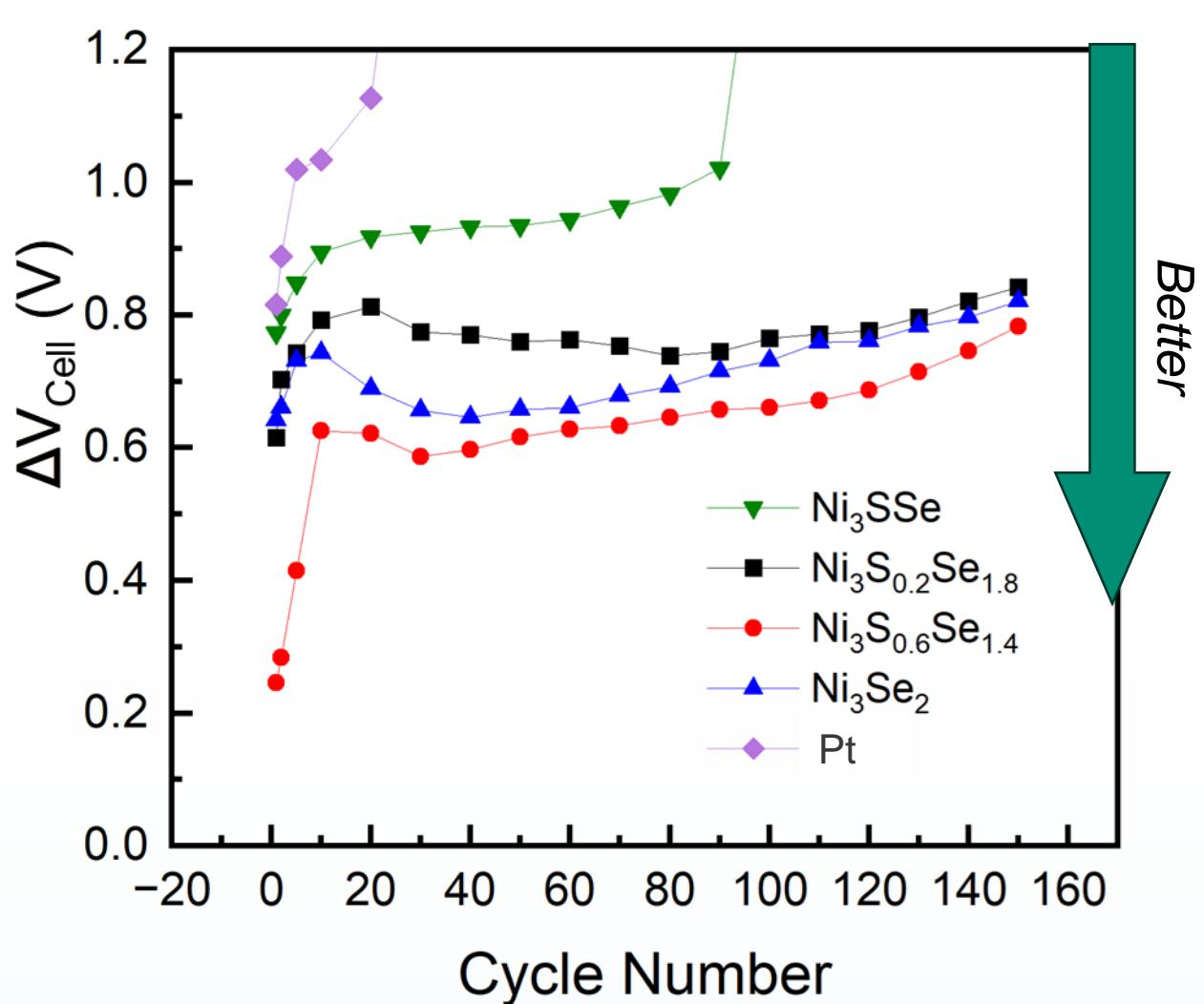


Synthesis of Metal Chalcogenides

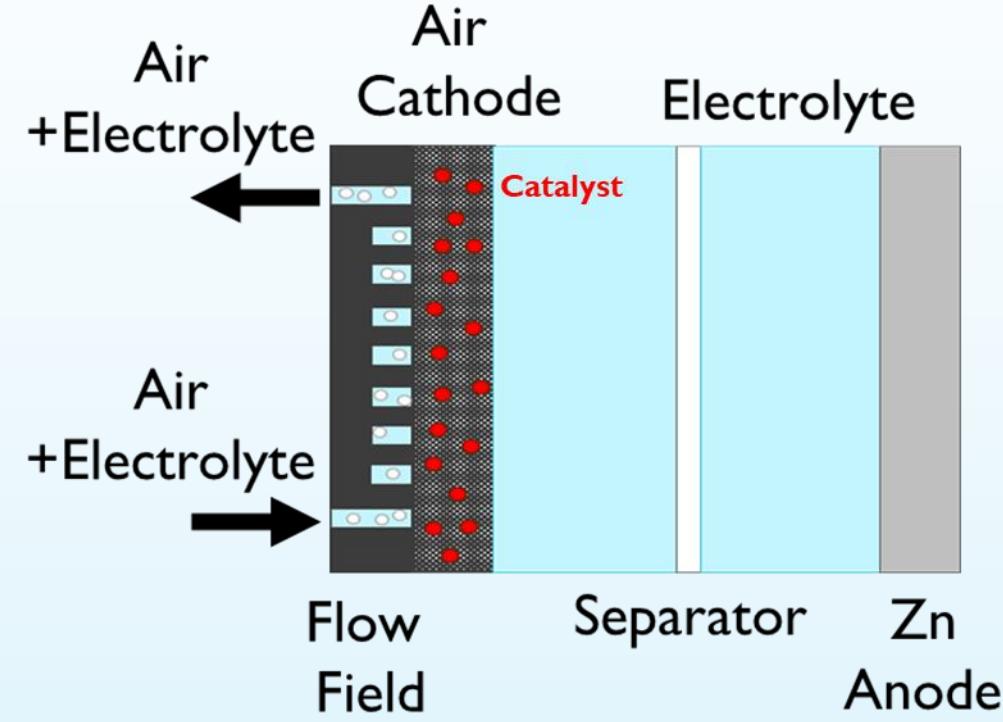


Using both hydrothermal and colloidal methods, we are able to synthesize different phase pure metal sulfoselenides (M= Ni, Mn) with variable concentrations of selenium and sulfur.

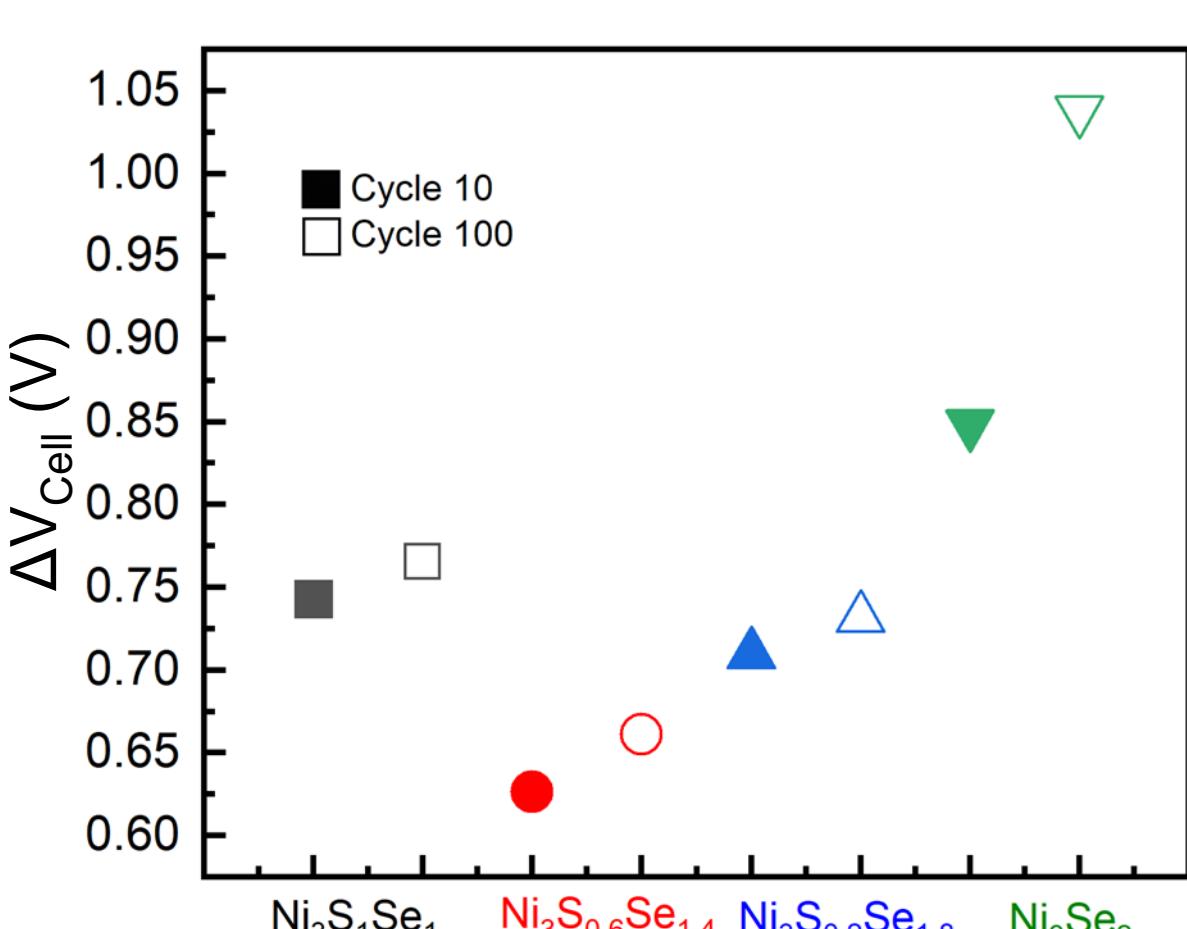
Flowing NiSSe Zn-Air Batteries



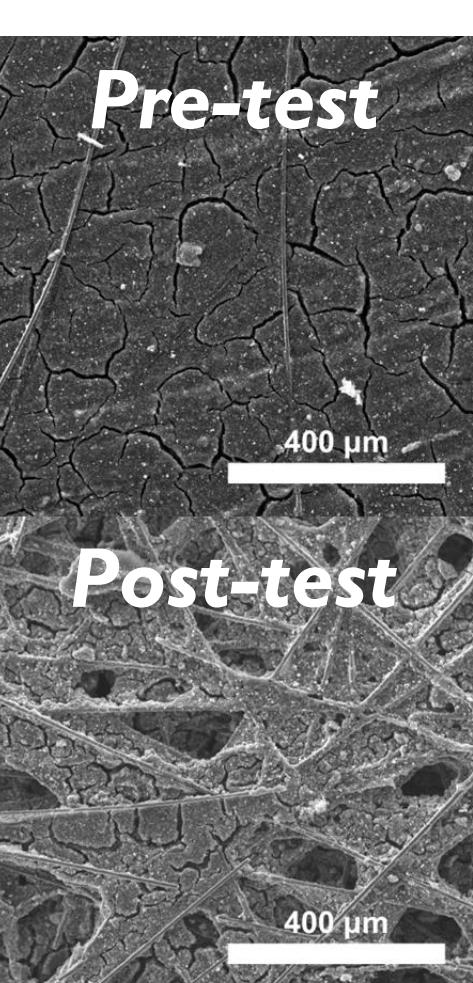
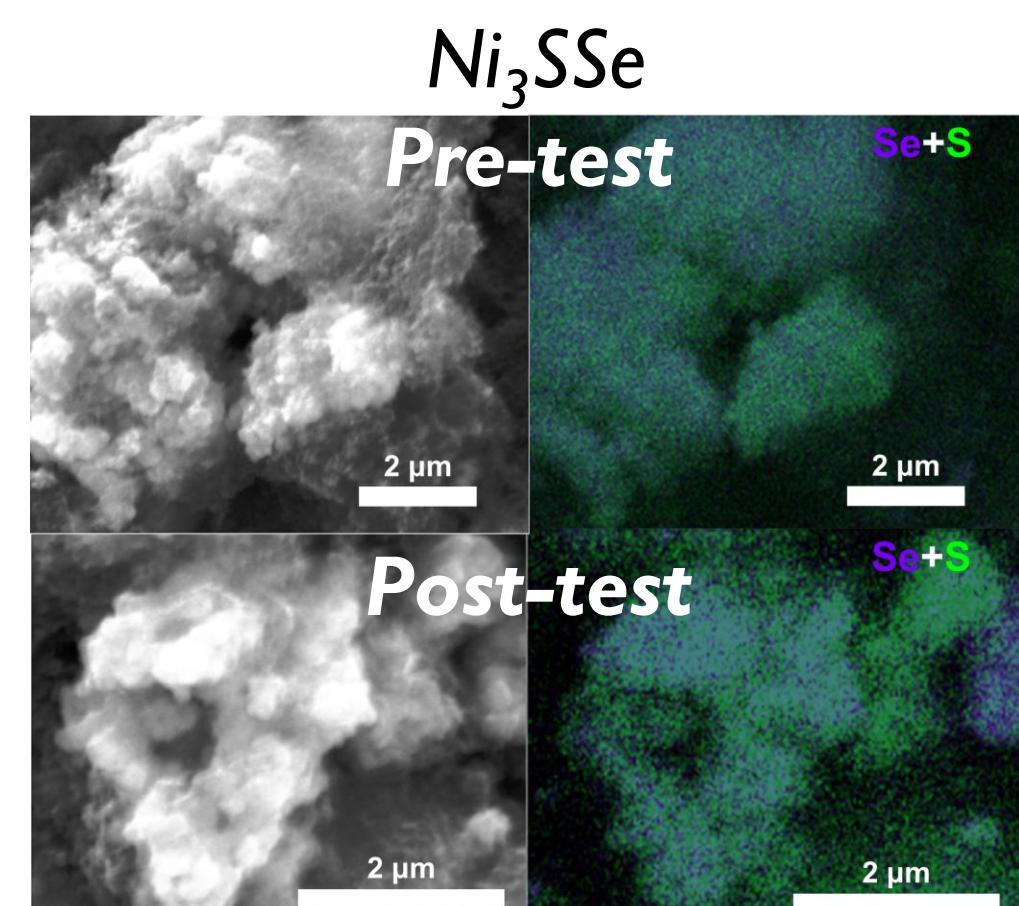
- When tested in air (not pure O₂), all NiSSe out-performed Pt/C
- $\Delta V_{Cell} = V_{Chg} - V_{Dis}$, measure of **overall** catalyst performance, is *lower* for moderate S incorporation
- Energy efficiency is *higher* for moderate S incorporation



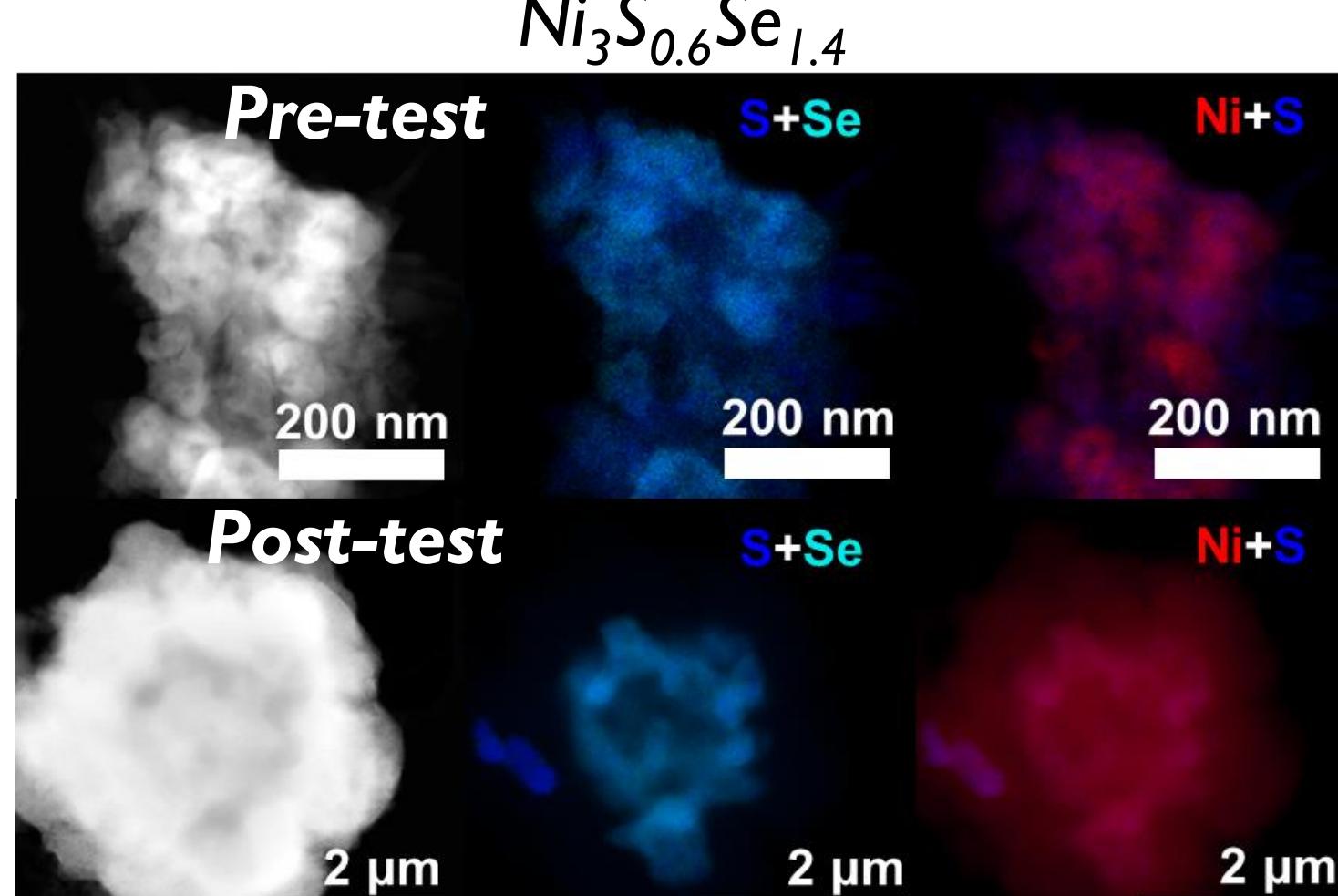
Stability of NiSSe Electro catalysts



Mixed chalcogenides exhibit less voltage fade with cycling

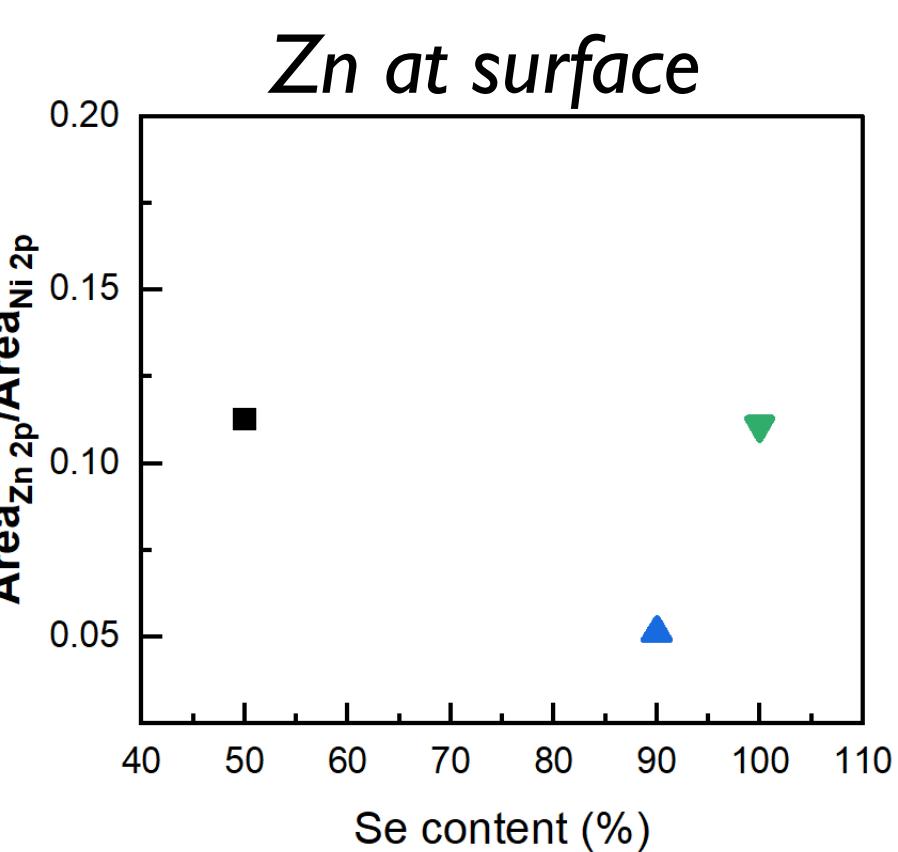
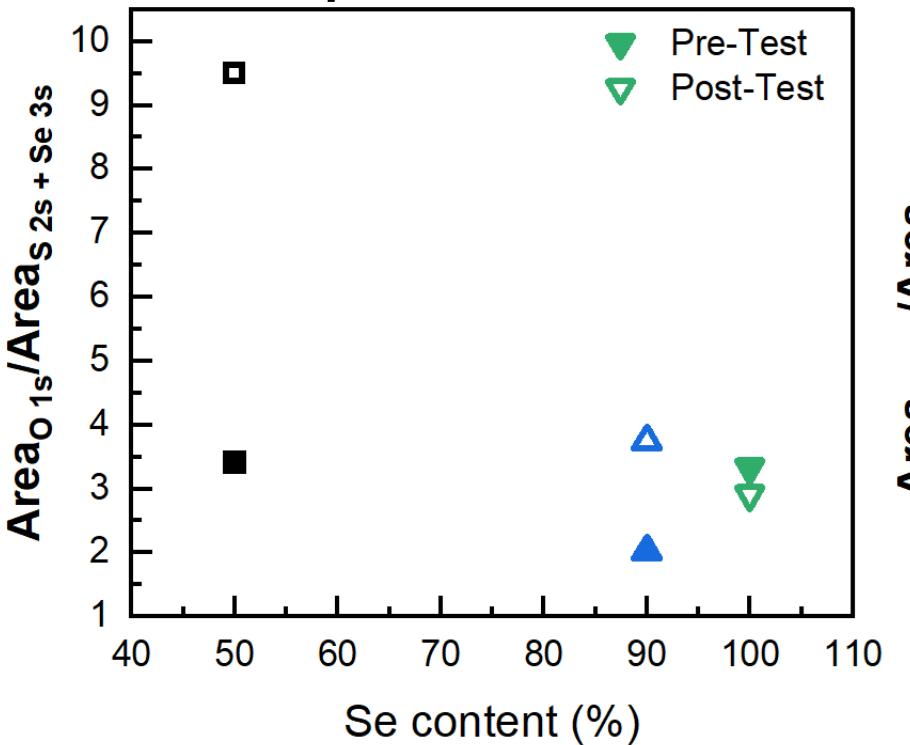


Both S and Se are lost from the NiSSe surface after battery cycling, although a core remains



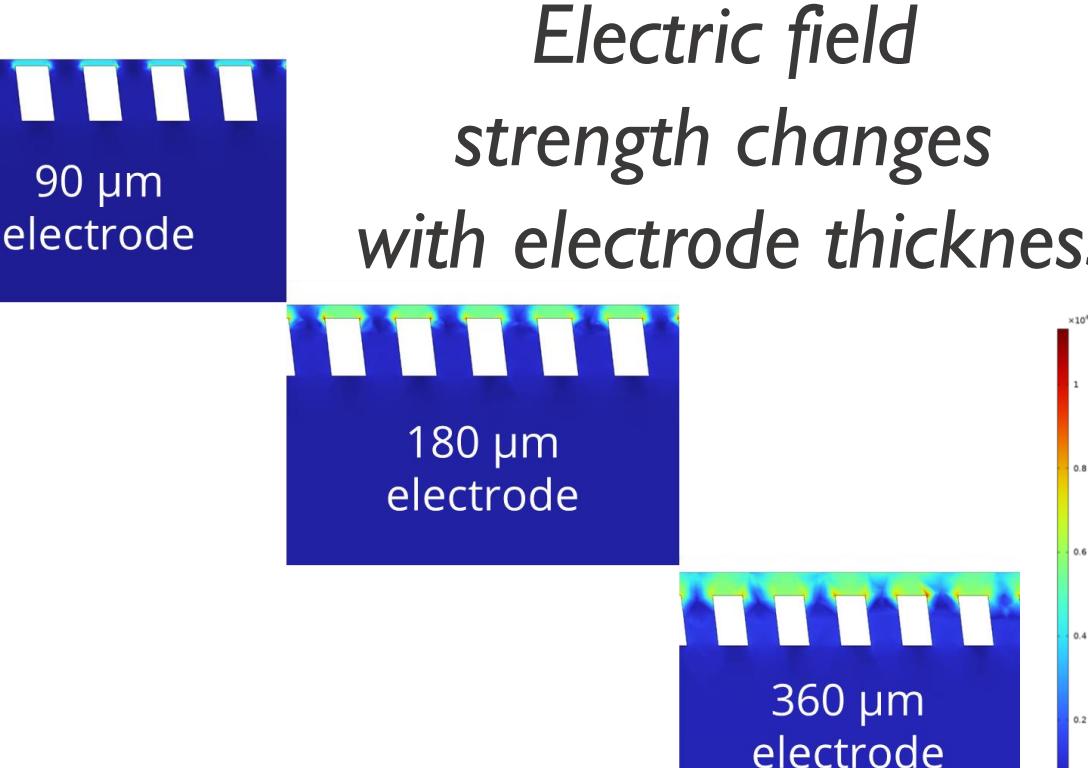
Physical Loss of Material with Cycling

Surface Oxidation

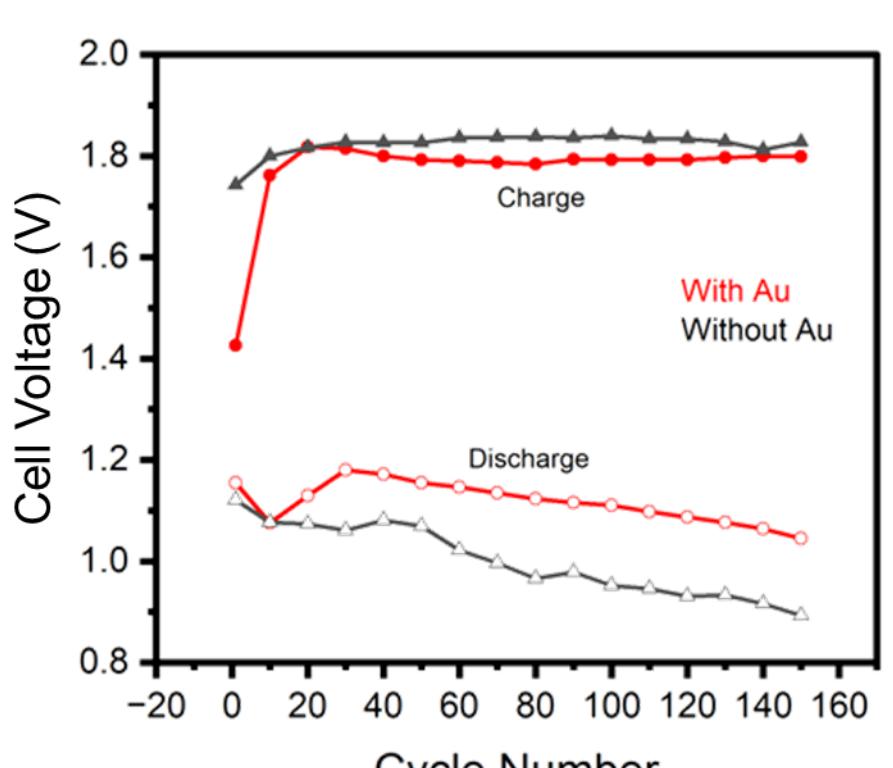


X-ray photoelectron spectroscopy (XPS) confirms a) NiSSe surface oxidation trends with Se content and b) Zn is adsorbed to the electrode surface

Electric Field Modulation with Au



- Au can be added to the electrode to help control electric field
- Improves discharge voltage, but more study needed to determine how



Conclusions + Future Directions

- NiSSe BOEs can be used with the SNL fZABs, and demonstrate better performance than Pt/C through S/Se tuning.
- Moderate S incorporation in Ni₃Se₂ shows best performance and stability
- Decreased performance over time could be due to: a) Loss of catalyst, b) excessive catalyst oxidation, c) surface fouling with Zn
- Adding a small quantity of gold to the electrode improves performance by 10%

What next?

- Test the cells for longer periods of time with higher capacity cycles
- Development of Mn-based sulfoselenides to replace Ni
- Understanding why gold improves performance of NiSSe