Sandia National Laboratories

IRON SULFOSELENIDE NANOPARTICLES AS TUNABLE BIFUNCTIONAL OXYGEN ELECTROCATALYSTS

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PROJECT PROFILE

Topic: Zn & Pb Batteries| Vertical: Materials Innovation

Strategic Pathway: Enabling innovation and advancing new technologies

Project start and finish: FY25-FY26

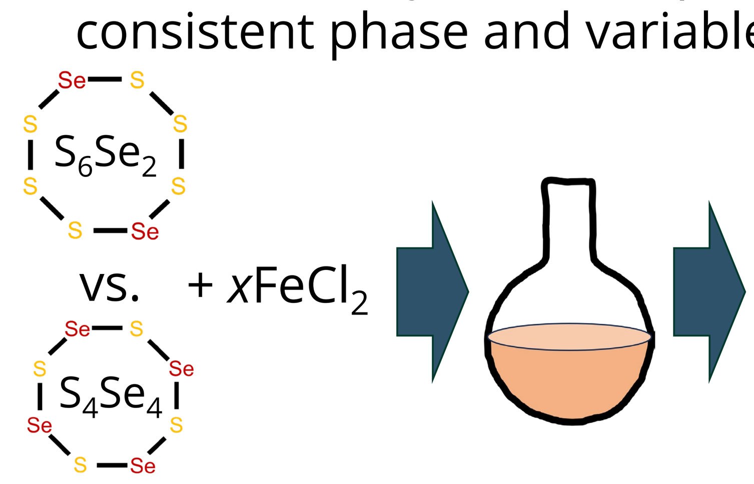
PROBLEM

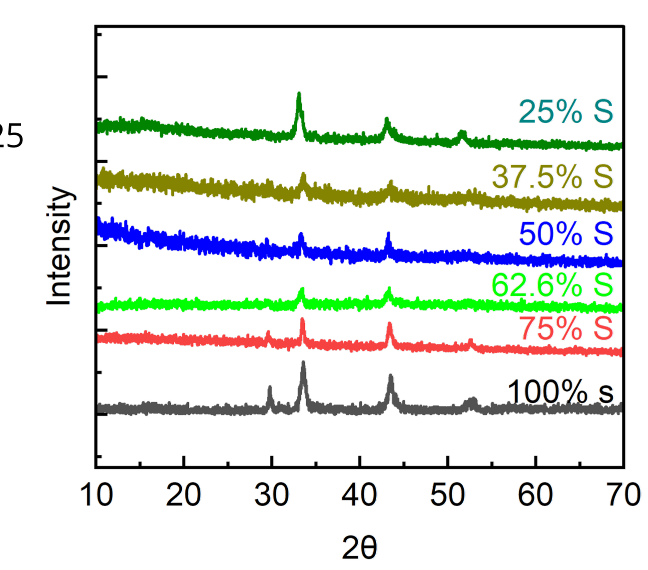
- Li-ion batteries ideal for applications where energy and power density are required, but stationary storage emphasizes cost and safety
  - Focus on earth-abundant materials, domestic supplies
- Zn-air batteries represent a promising alternative with high theoretical energy density, but are typically primary cells with low voltage
  - Efficient, stable, inexpensive electrocatalysts needed to improve cathode performance; replace precious metals
  - Bifunctional Oxygen Electrocatalyst (BOE) for charge/discharge
- Metal sulfoselenides (MSSe) are promising candidates due to tunable (electro)chemical properties using S/Se composition
- **Iron sulfoselenides** (FeSSe) represent a lower-cost alternative to Ni

APPROACH

Synthesis

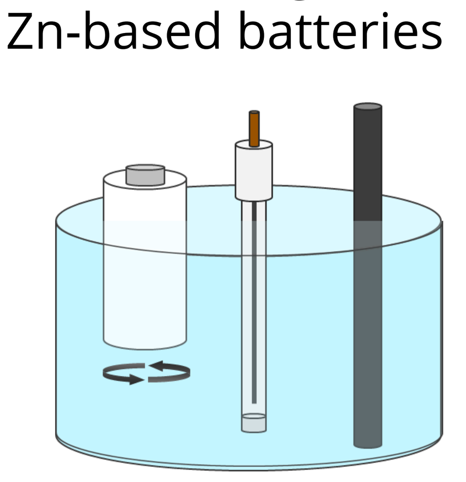
1. Create cyclic S-Se compounds as precursors with tunable S/Se ratios
2. Use colloidal synthesis to prepare $Fe_7S_{9-y}Se_y$ nanoparticles with consistent phase and variable S/Se ratios



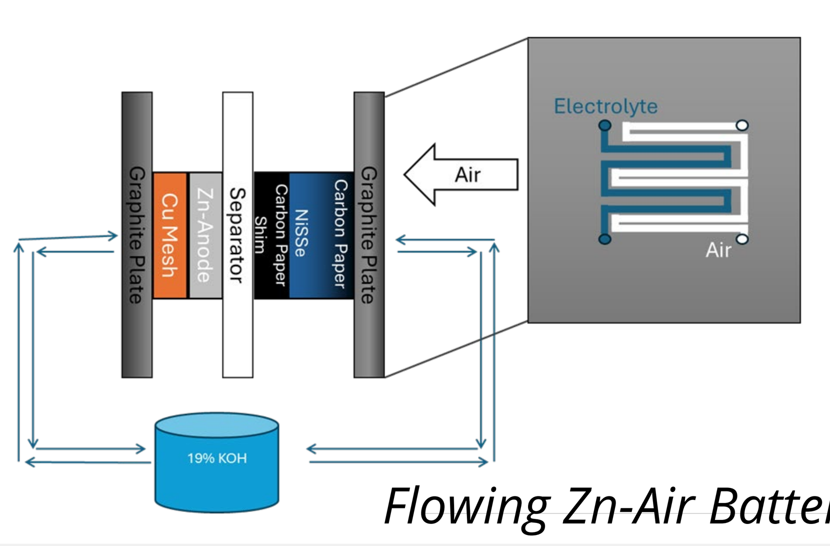


Characterization

1. Physiochemical characterization of FeSSe electrocatalysts allows phase, size, composition, and surface/bulk chemistry to be studied
2. Electrocatalytic testing using a rotating disk electrode (RDE) and cyclic voltammetry (CV) allows quantification of electrocatalyst performance
   1. Oxygen Evolution Reaction (OER)
   2. Oxygen Reduction Reaction (ORR)
3. Work leverages SNLs prior experience with MSSe electrocatalysts and Zn-based batteries



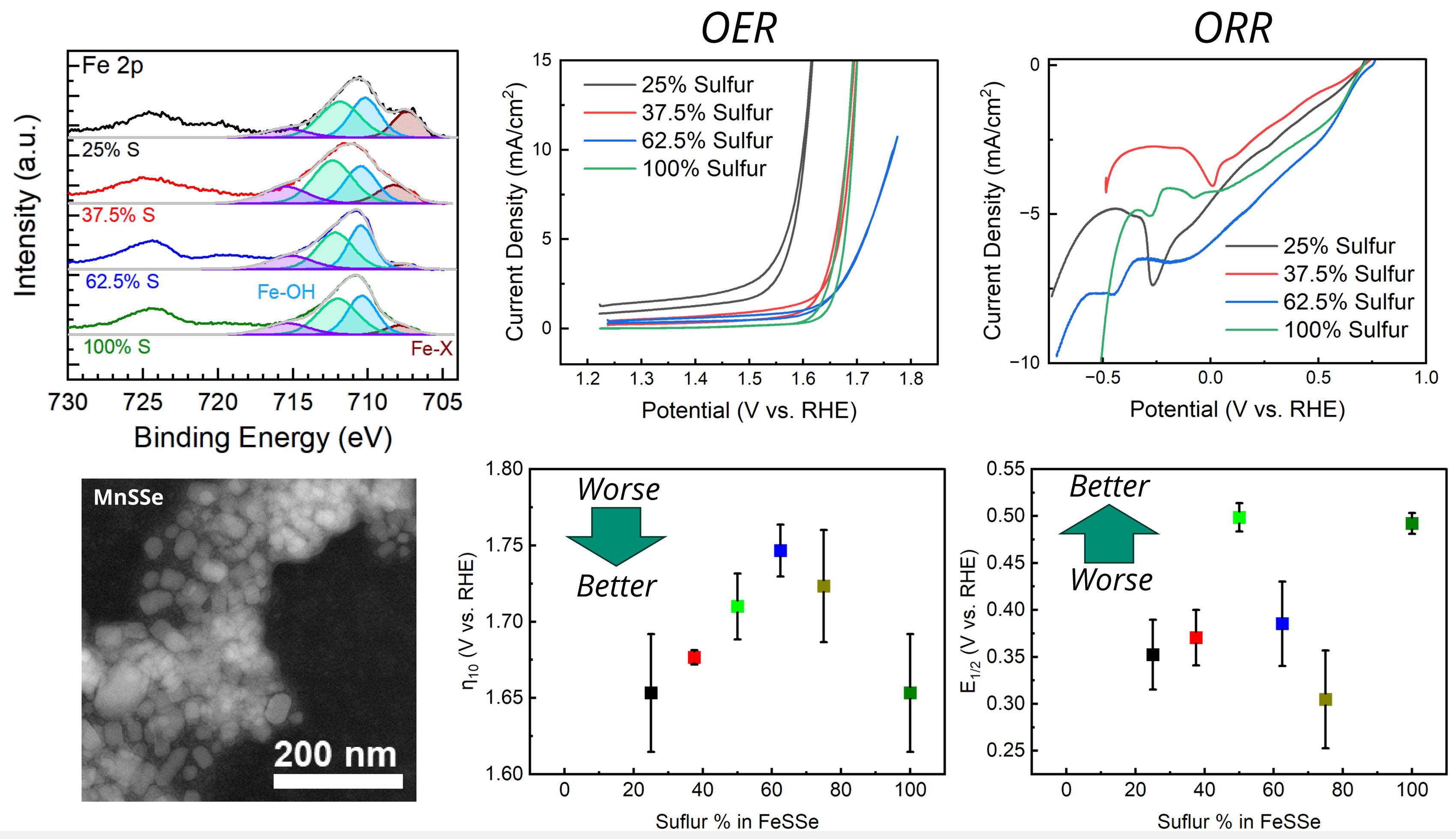
3-Electrode RDE Cell



Flowing Zn-Air Battery

RESULTS

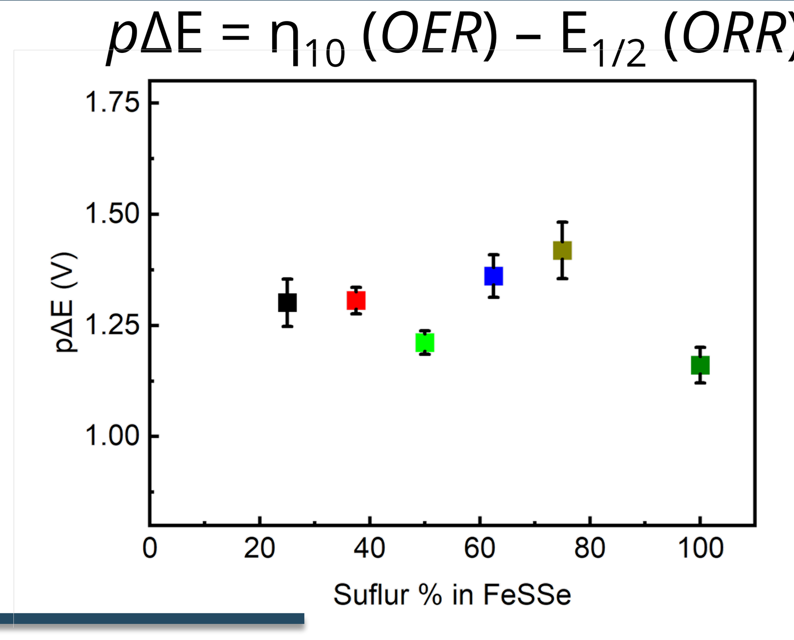
- X-ray photoelectron spectroscopy (XPS) indicates reduced Fe in FeSSe
- FeSSe particles are likely ~50-100 nm (similar to MnSSe measured by scanning transmission electron microscopy, STEM)
- CV shows that OER is influenced by S/Se, but ORR is less affected



CONCLUSIONS & IMPACT

1. Colloidal synthesis can be used to synthesize phase pure FeSSe
2. Similar to NiSSe, S/Se ratio does have an impact on OER/ORR behavior
3. Fe_7S_8 currently best, but $Fe_7S_4Se_4$ also shows promise

$$p\Delta E = \eta_{10}\,(OER) - E_{1/2}\,(ORR)$$



- FeSSe BOEs could be much less expensive (~175%) than NiSSe or Pt
- Single electrocatalyst for OER and ORR simplifies battery design
- OER and ORR electrocatalysts can be applied to many energy technologies
  - Electrolyzers, fuel cells, electrochemical synthesis

FUTURE DIRECTIONS

1) Complete detailed physiochemical characterization of FeSSe precatalyst before and after OER/ORR to understand how electrochemistry influences the final electrocatalyst
2) Integrate promising FeSSe electrocatalysts into Zn-air batteries to evaluate performance as an air cathode
3) Synthesize quarternary FeNiSSe precatalysts to improve BOE performance

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