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TRANSITION METAL MULTICHALCOGENIDES AS BIFUNCTIONAL OXYGEN ELECTROCATALYSTS FOR ZINC-AIR BATTERIES

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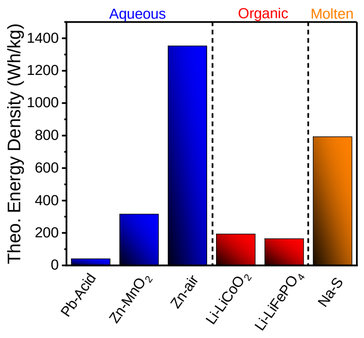
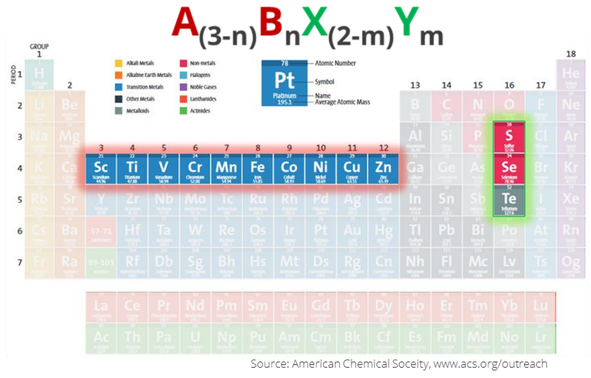
Background

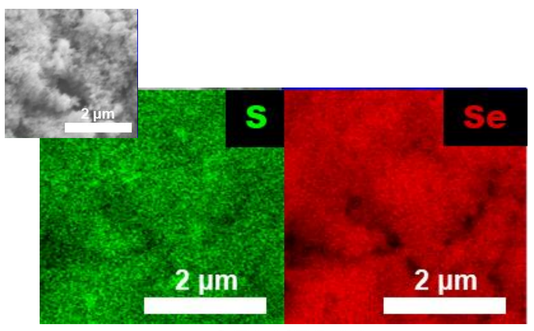




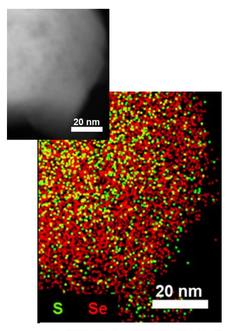
- Zn-air (and other metal-air chemistries) are viable alternaitves to Li-ion batteries, but require better bifunctional oxygen electrocatalysts (BOEs) to replace precious metals like Pt and Ru
- Transition metal chalcogenides have demonstrated good performance as oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) electrocatalysts and have a broad degree of chemical "flexibility", making them excellent targets for further research

Synthesis and Characterization

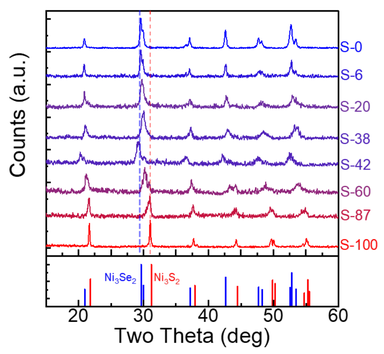
- Hydrothermal reaction to produce series of $Ni_3S_{2-x}Se_x$ (NiSSe) powders



SEM/EDX



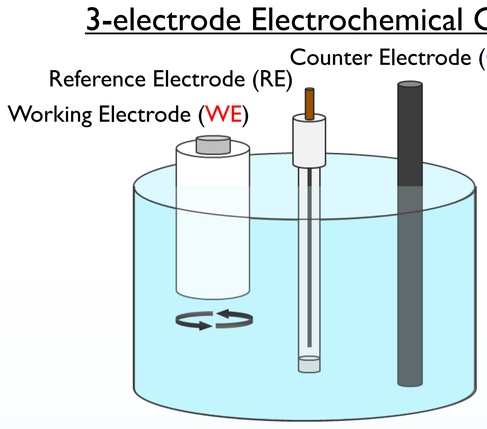
STEM/EDX



- Characterization shows that the materials show a transition from Ni_3S_2 to Ni_3Se_2, but that the S/Se in the material is evenly distributed within discreet particles

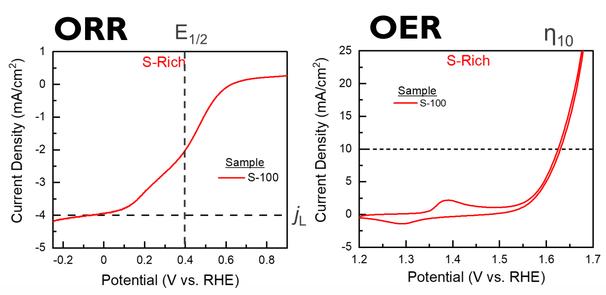
Electrocatalytic Testing

3-electrode Electrochemical Cell



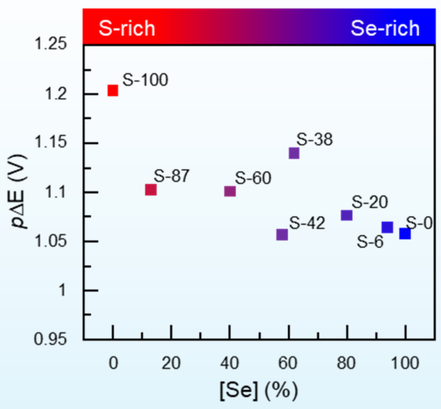
WE : $4\ OH^- \rightarrow O_2 + 2\ H_2O + 4\ e^-$ (OER)

CE : $4\ e^- + 4\ H_2O \rightarrow 4\ OH^- + 2\ H_2$ (HER)



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

BOE OER ORR



- Electrocatalytic testing in 3-electrode cells allows testing for OER and ORR performance, as well as determination of $p\Delta E$, a measure of BOE performance

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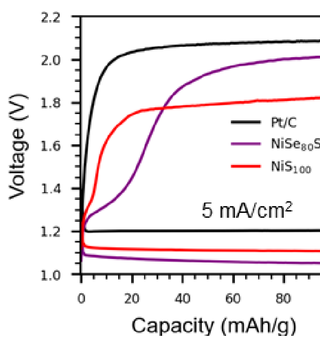
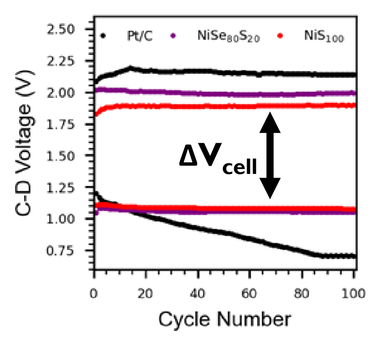
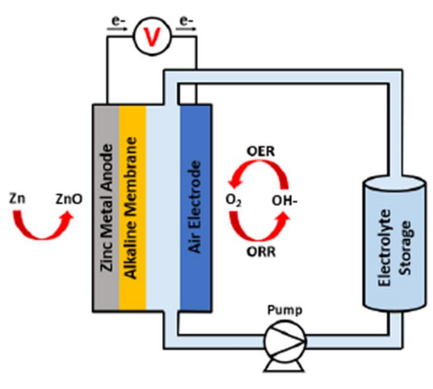
Zn-Air Battery Performance

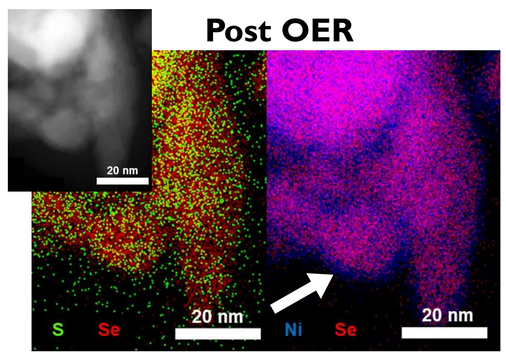
- Testing in a flow Zn-air battery shows improved BOE performance for NiSSe compared to commercial Pt/C

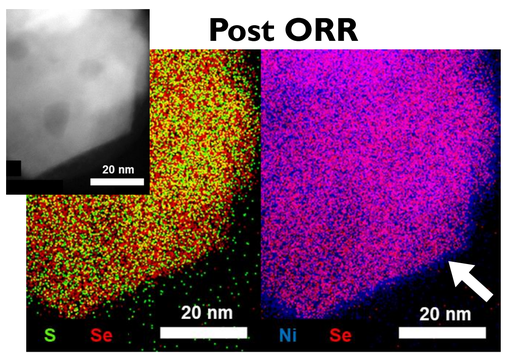






Controlled Surface Oxidation

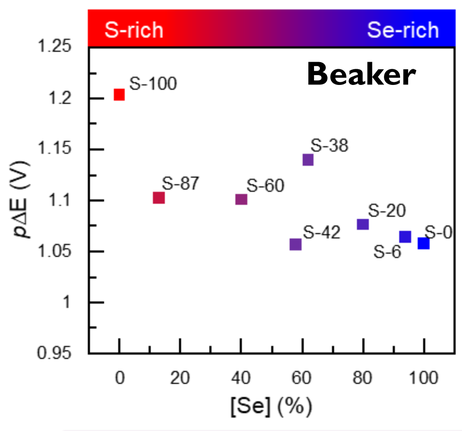




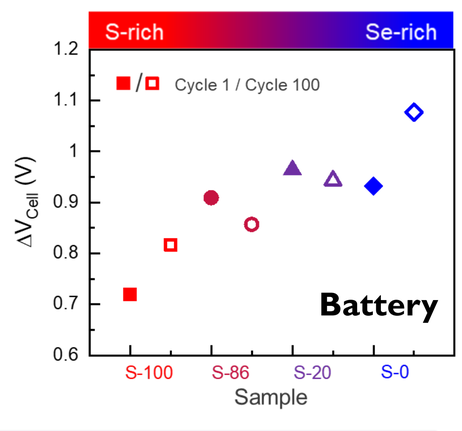
- STEM EDX mapping shows that the surface of NiSSe after OER and ORR consists of a thin O-rich layer atop the S/Se bulk, likely active electrocatalyst
- S is more readily oxidized, Se is more stable and more conductive; mixing them helps generate optimal material for BOE

Differences in Beaker vs. Battery

- For limited tests in batteries, the trend for overall BOE performance is inverted; Se-rich appear to be *worse* BOEs



vs.



Conclusions + Future Directions

1. Hydrothermal synthesis is a simple, tunable method for producing mixed metal chalcogenides
2. Electrocatalytic performance of NiSSe materials is promising, and suggests that Se-rich materials may be suitable BOEs for Zn-air batteries

BUT

1. A better understanding of why BOE trends differ for 3-electrode tests and batteries is needed to help drive further research
2. Exploration of more earth-abundant metals (e.g., Fe) will help further improve costs for developing and building Zn-air batteries

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