Development of Solid-State Li/Sulfur-Selenium as Safe and High Capacity Battery

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Outline

- Introduction/NASA Energy Requirements
- Why Li/S-Se Chemistries
- Challenges for Developing Safe and high Capacity Li/S-Se Batteries
- Result Summary
- Next Steps

Safe and High Capacity Batteries: Important for NASA Missions

- **Batteries provide**
  - a versatile, reliable, safe and portable energy source, and are an essential component of the power system of virtually all NASA missions
  - Electrical energy storage options for NASA Space missions, such as:
    - Power during spacecraft eclipses
    - Peaking power for high power needs

- **Aeronautics**
  - Electrified Aircraft (EA)
  - Urban Air Mobility (UAM)
- **Space**
  - Moon to Mars and beyond

Desired Battery Properties for NASA Missions

- Safe
- High in specific energy
- Light in weight
- Compact in volume
- Long in shelf life
- Durable in wide temperature ranges and harsh environments
- Reliable in meeting mission requirements

State-of-Art (SOA) Li-Ion Battery (LIB)

- **LIB Specs**:
  - Specific energy: 180-200 Wh/kg
  - Specific power: 300 W/kg
  - Cycles: 1000s (excellent)
  - Temp range: -20^{o}C to 60^{o}C
  - Excellent rechargeability

- **Limitations**:
  - Maximum of energy density <250 Wh/kg
  - Electrolyte flammable and fire hazards

NASA Demands Very High Specific Energy Batteries

Electric Aviation

500 – 750 Wh/kg

- Green aviation – Less noise, lower emissions, high efficiency
- Hybrid / All-electric aircraft – Limited by mass of energy storage system
- Commercial aviation – Safe, reliable, lightweight on-board electric auxiliary power unit

Extravehicular Activities (Spacesuit power)

>400 Wh/kg

Required to enable untethered EVA missions lasting 8 hours within strict mass and volume limitations.

- Astronaut life support
- Safety and reliability are critical
- 100 cycles

Landers and Rovers, Robotic missions, In-space habitats

>500 Wh/kg

Batteries are expected to provide sufficient power for life support and communications systems, and tools including video and lighting

- >100 cycles

NASA future mission requirements far exceed the capabilities of SOA Li-ion chemistries

➢ Progress in these areas requires advances in safe, very high energy batteries

Li/S – Potential High Energy Battery Chemistry

- Lithium (Li) metal: High capacity anode (3860 mAh/g)
- Sulfur (S): high capacity cathode (1670 mAh/g)
- Li/S battery: high theoretical specific energy: 2680 Wh/kg
- Low cost and availability of sulfur
- Non-toxic
- Environmentally benign

Li/S – Challenges

- **Poor intrinsic electronic conductivity of sulfur (S)**
  - **1 x 10^{-18} S/cm**
  - **sluggish kinetics and poor power capability**
- **Polysulfide shuttle (PS) - short cycle life**
- **Li dendrite growth – safety concern**

Li/S – Approaches to Overcome Key Issues

- **Improve Electronic Conductivity of Sulfur Cathode**
  - Carbon (C) conductive additives for C/S composite
    - Various carbons
    - Holey graphene (developed from NASA Langley)
  - Seleniu(Se)/Selenium compounds (SeS_x)
    - as active materials and higher electronic conductivity

- **Reduce/Eliminate Polysulfide Shuttling (PS)**
  - Porous carbon to confine S in the pore
  - Surface coating on separator to block PS migration
  - Solid state electrolyte to eliminate PS

- **Improve Safety by Developing Safe Electrolytes**
  - Non-flammable electrolyte -->eliminating fire hazard
  - Solid polymer composite electrolyte --> improving safety/PS
  - Solid state electrolytes (sulfide-based, oxide-based….)
    -->addressing safety and PS issues

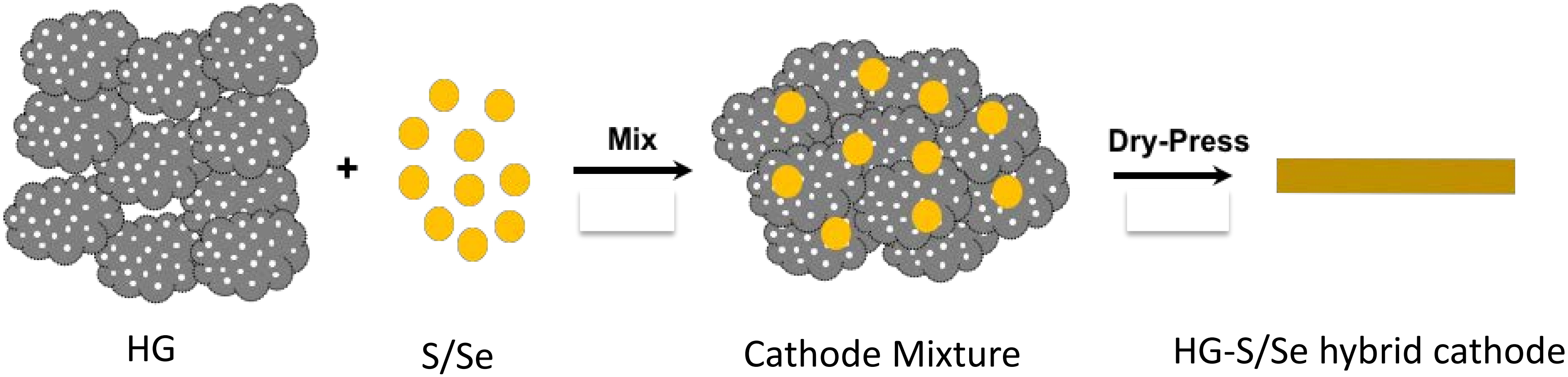
Hybrid Sulfur Cathode: Active Components

Component	Electronic Conductivity (S/cm)	Theoretical Capacity (mAh/g)
S	1×10^{-18}	1675
Se	1×10^{-5}	678
SeS_2		1123

Introduction of Se or Se compound in S cathode:

- **both active material and better electronic conductivity**
- **improve cathode overall electronic conductivity**
- **ratio of S vs. Se to be optimized to maximize the energy and power densities**

Hybrid Sulfur Cathode: Holey Graphene (HG) as Host

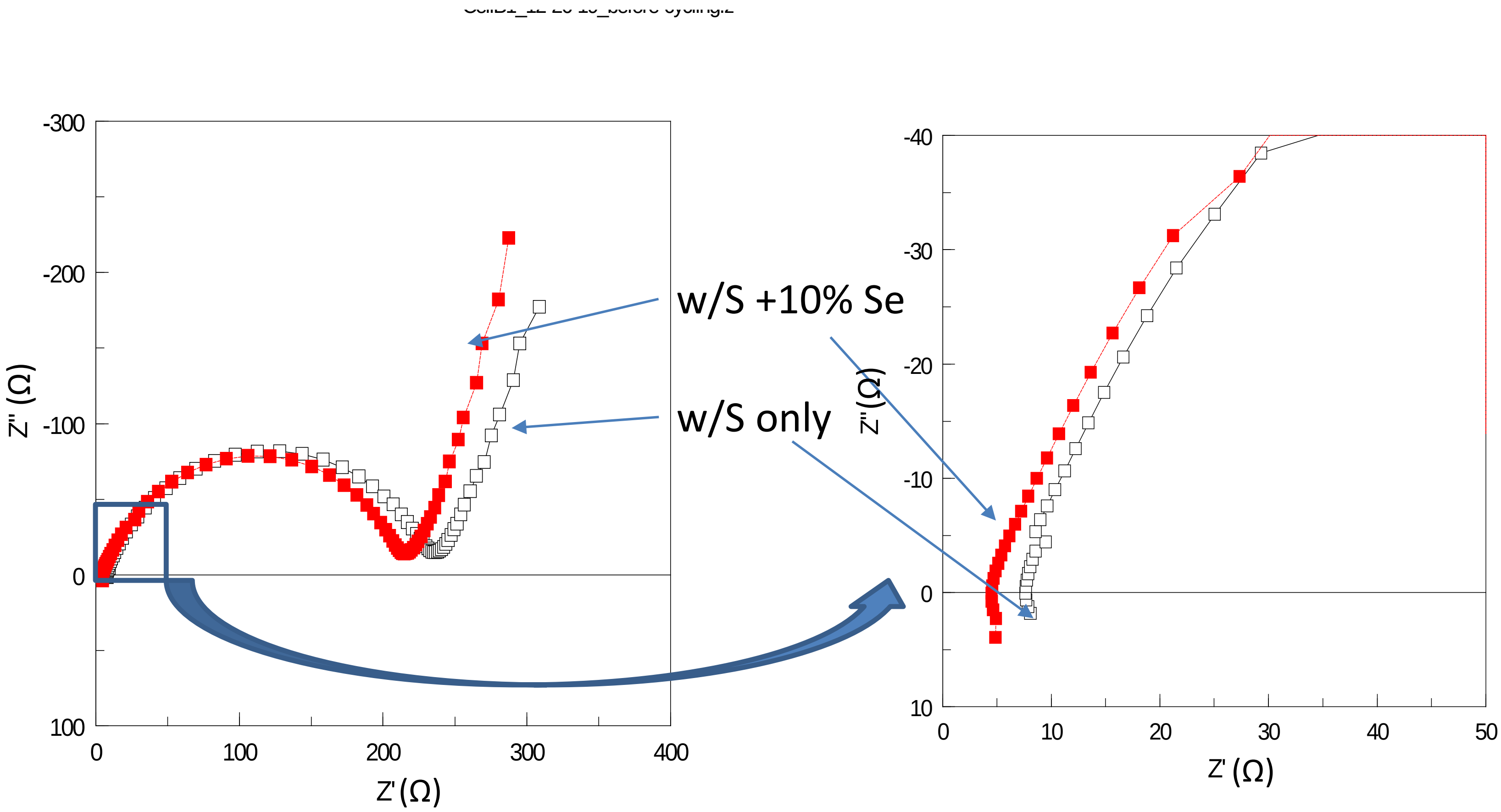


Advantages of Holey graphene:

- Highly conductive
- Ultralight weight
- Easy ion transport through the holes --> fast kinetics
- Dry-press (solvent-free) fabrication

S/Se Hybrid Cathode: Impact of Se

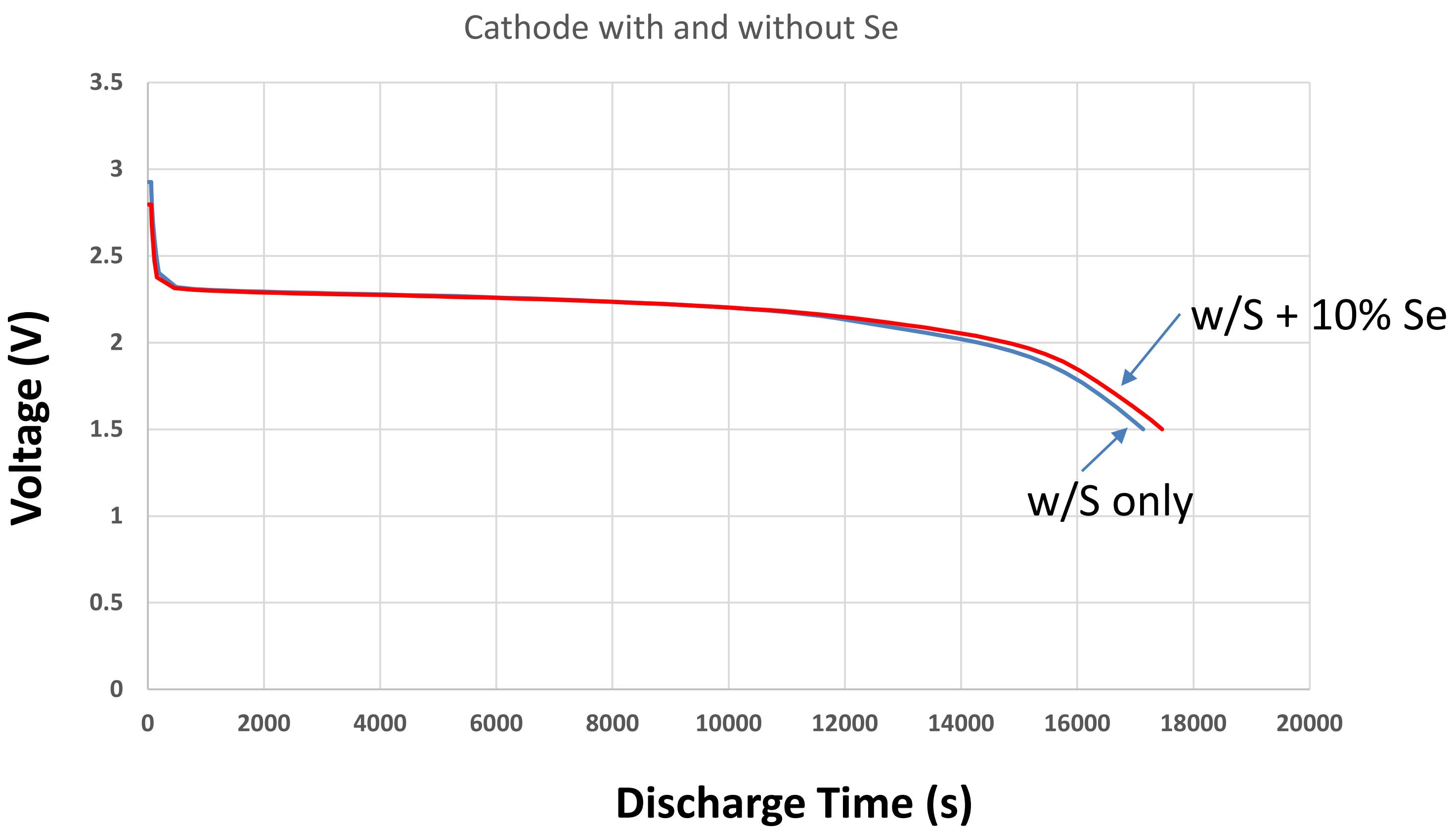
Cathode w/ and w/o Se on Initial Cell Impedance



Cathode w/10% Se improves the cell electronic conductivity

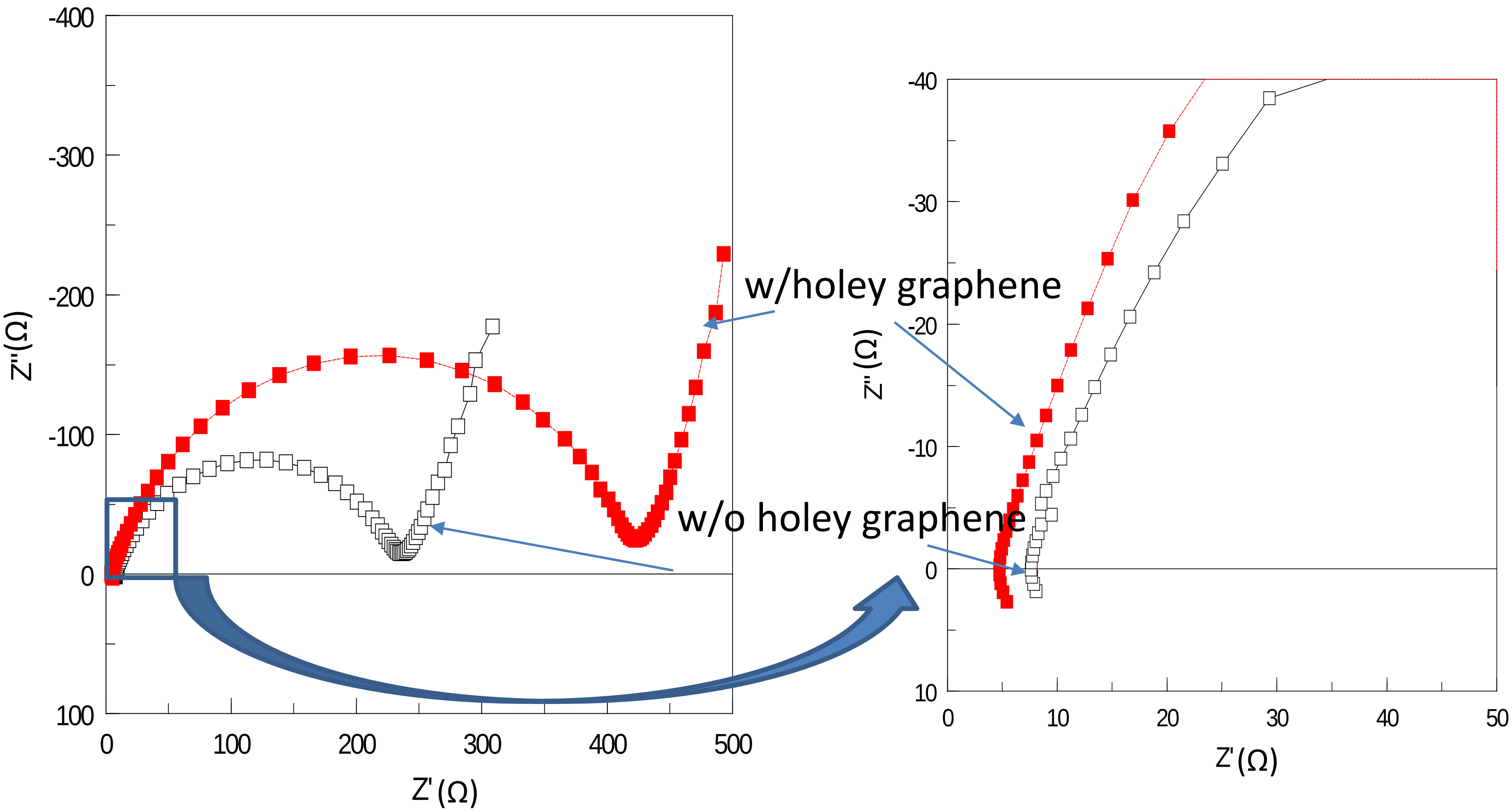
S/Se Hybrid Cathode: Impact of Se

Initial Discharge Voltage Profile of Cathode w/ and w/o Se



Introduction of Se enhances the utilization of S in the hybrid cathode

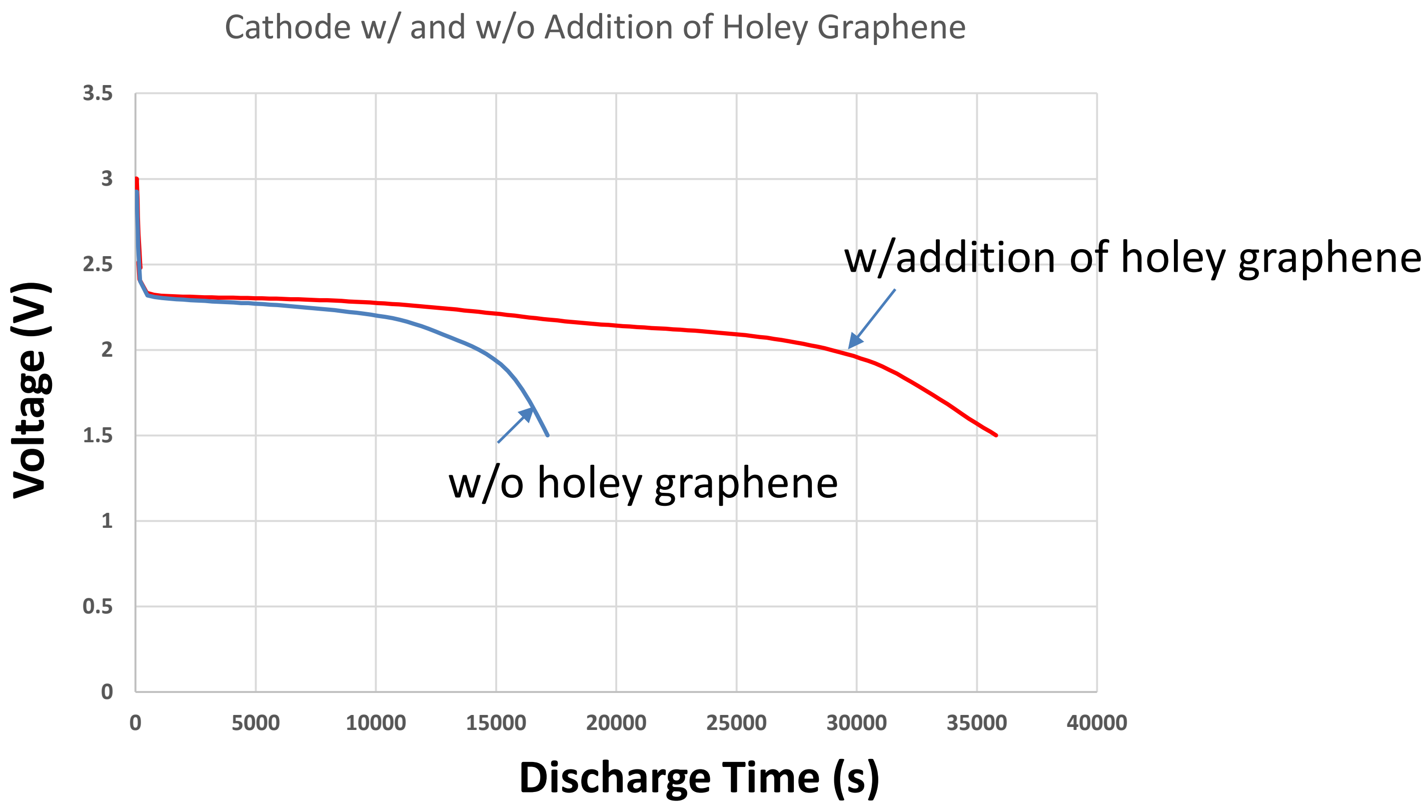
Sulfur Cathode: Impact of Holey Graphene



Addition of holey graphene improves cathode electronic conductivity

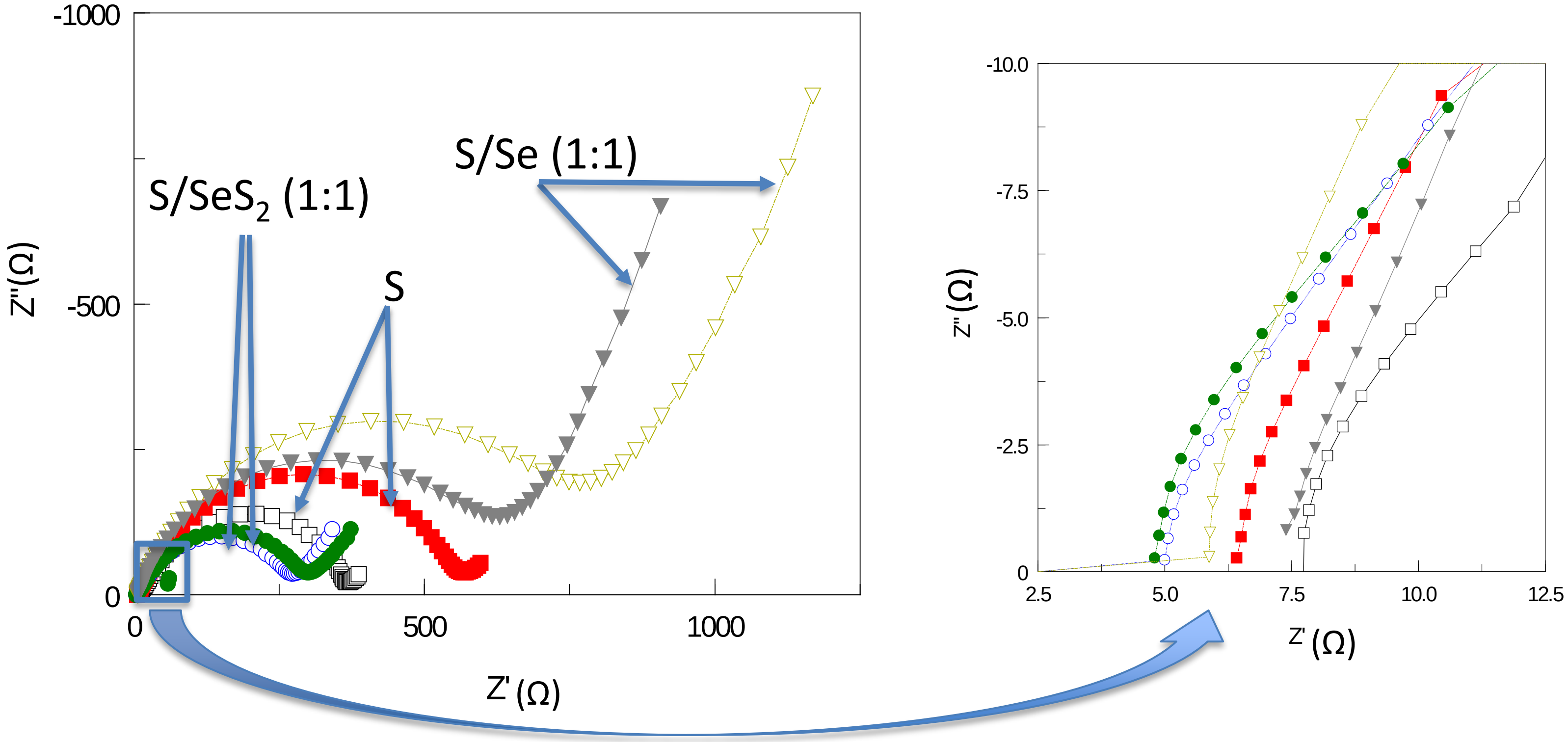
Sulfur Cathode: Impact of Holey Graphene

Initial Discharge Voltage Profile of Cathode w/ and w/o Addition of Holey Graphene



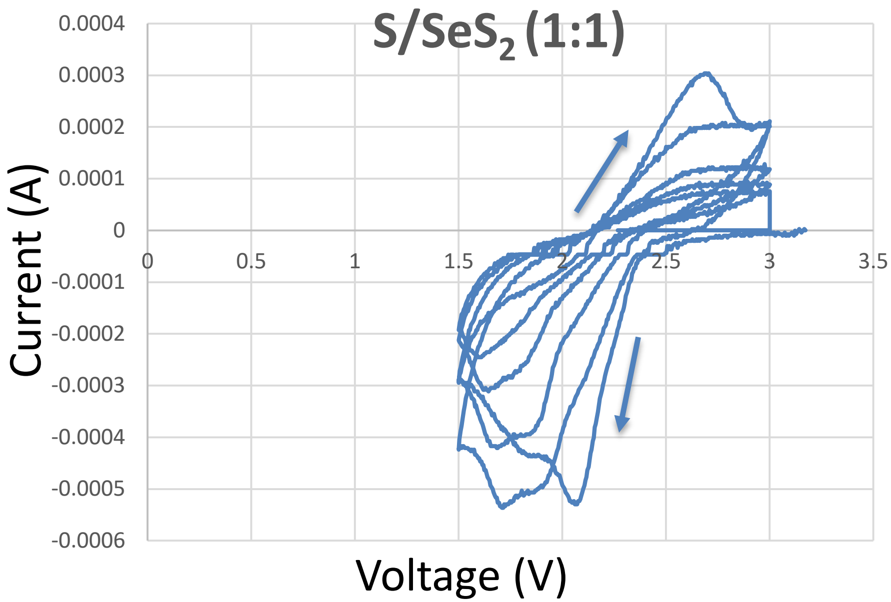
Addition of holey graphene significantly improve the initial discharge capacity

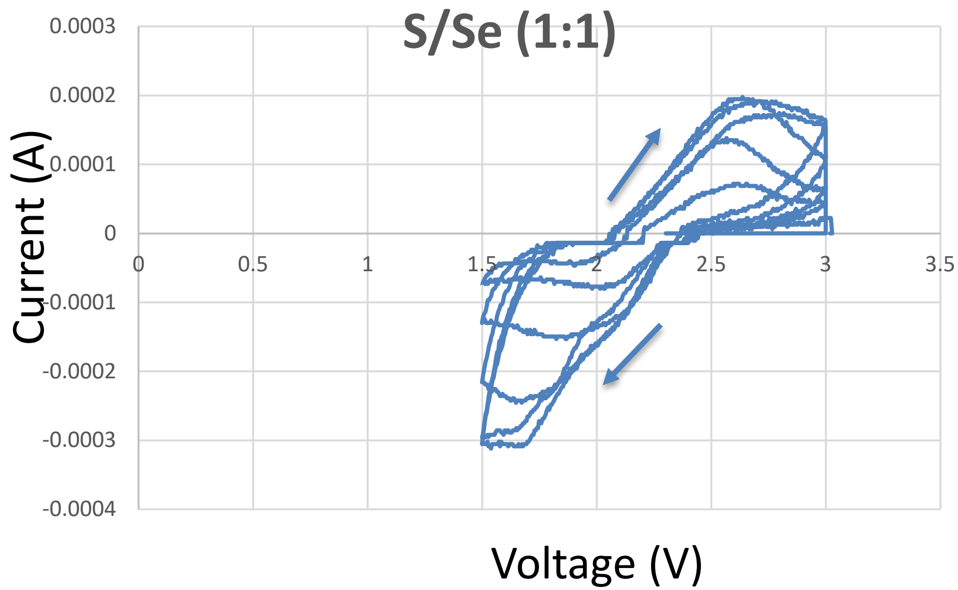
Hybrid Cathode: S/Se or S/SeS_2 vs. S

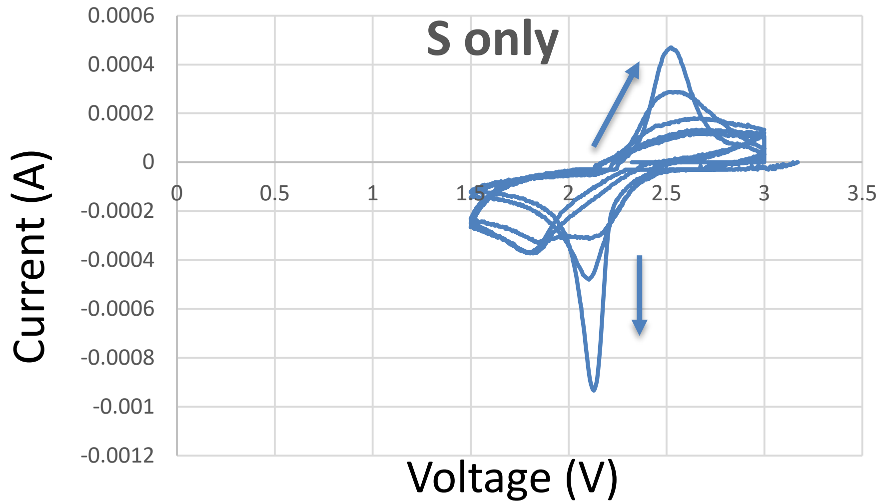


- **Cathode electronic conductivity: S/SeS_2 > S/Se > S**
- **Cell impedance: S/Se_2 < S < S/Se**

S/Se Hybrid Cathode: Cyclic Voltammetry



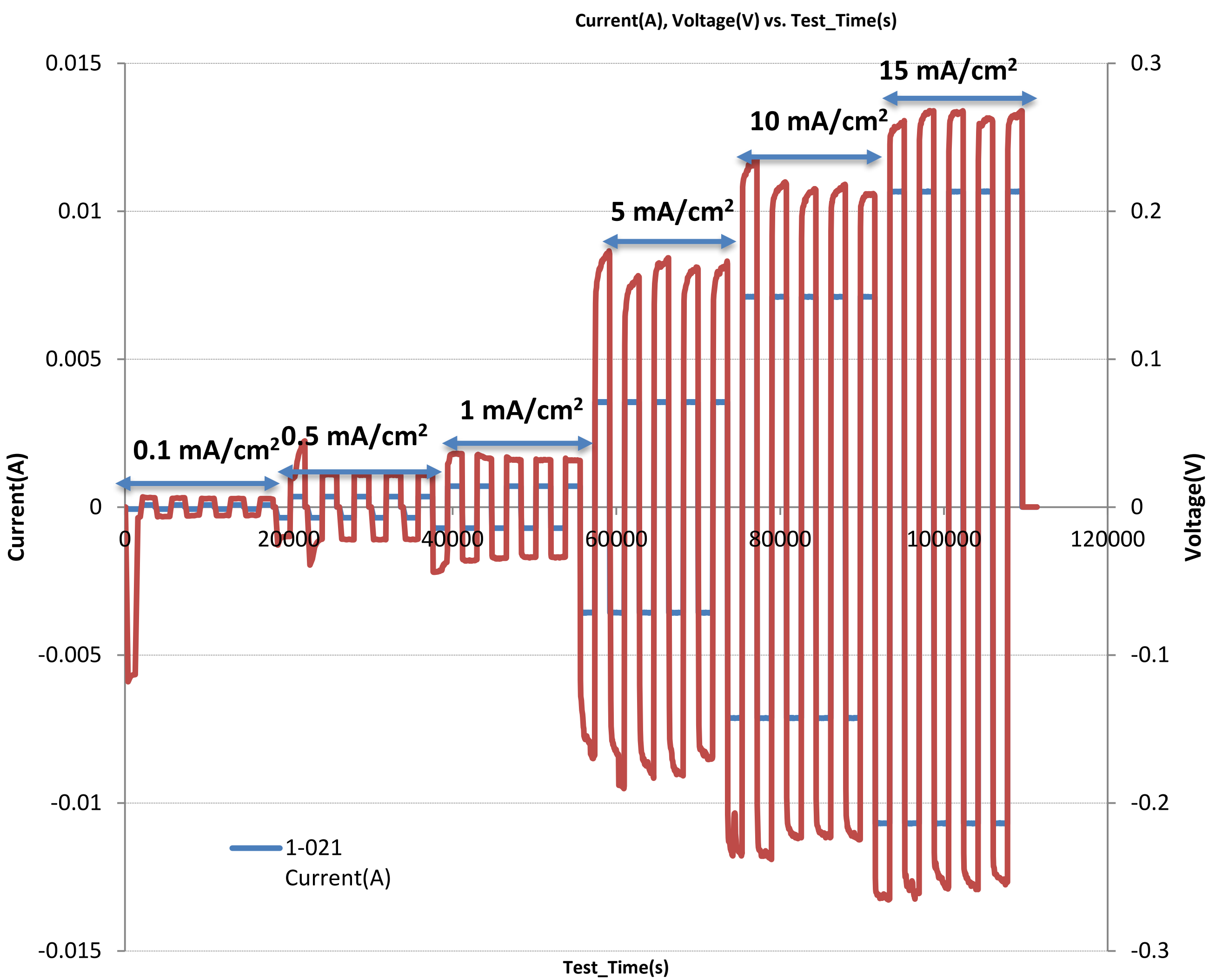




Solid Polymer Composite Electrolyte

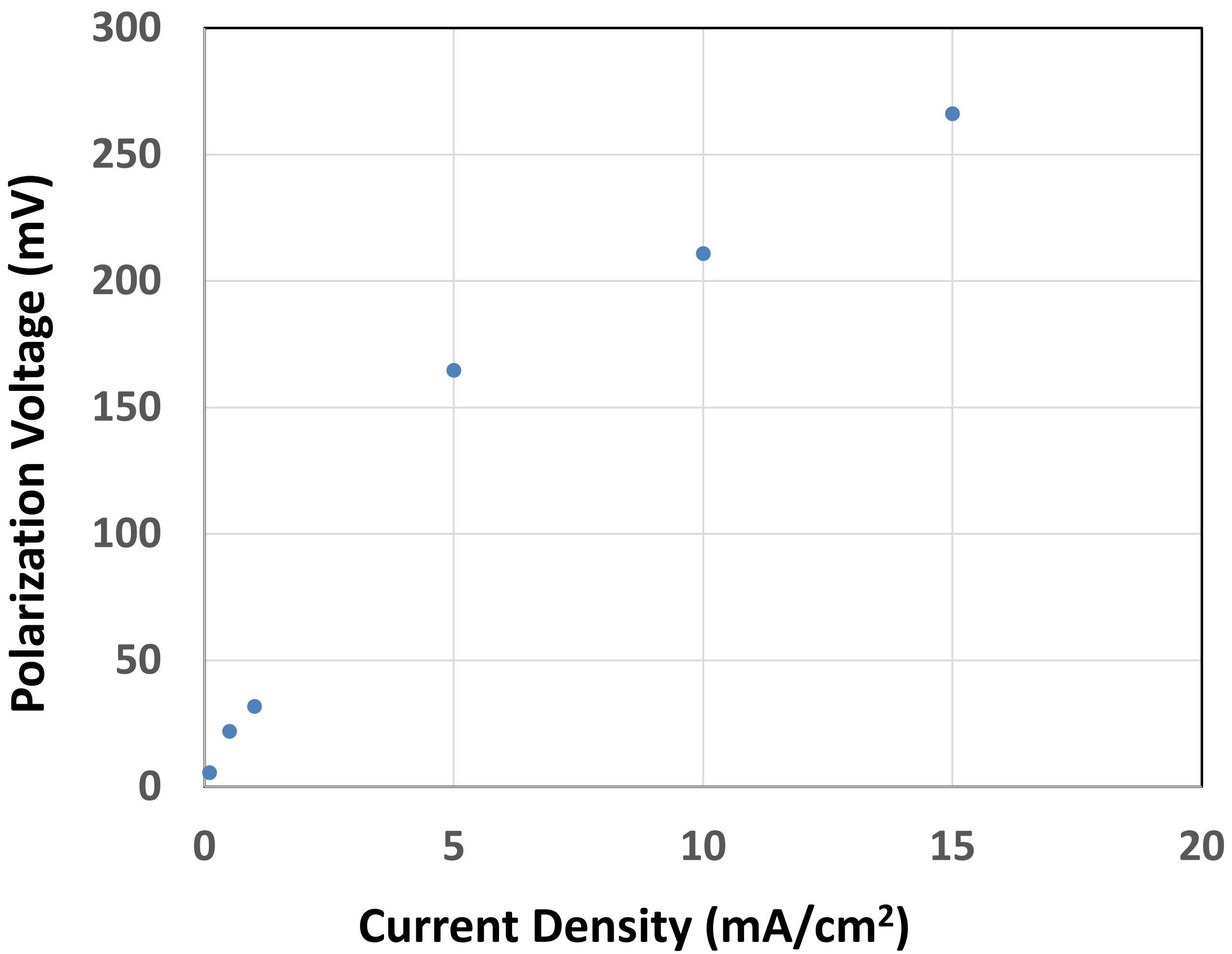
- **Polymer as host matrix, incorporating ceramic solid state electrolyte and Li salt**
- **Nonflammable, free-standing and flexible thin film**
- **Ionic conductivity: 1.2×10^{-3} S/cm**

Solid Polymer Composite Electrolyte: Various Current Densities at Li Symmetric Cells



It can take 15 mA/cm² current density

Polarization Voltage vs. Current Density (Li/Li Symmetric Cell)



Overall polarization voltage is low by the current, indicating polymer electrolyte/Li metal interface is well mitigated.

Summary

- **Addition of Se or Se compound to S reduces impedance and improves sulfur utilization**

- **Addition of holey graphene improves cathode electrical conductivity and the initial voltage discharge profile**

- **Nonflammable solid polymer composite electrolyte**
  - **Freestanding and flexible thin film**
  - **High ionic conductivity at RT**
  - **Capability to take high current density, indication Li metal/polymer electrolyte interface is stabilized/mitigated**
  - **Solid polymer nanocomposite electrolyte is an alternative and promising approach to enable Li metal cycling safely**

Current Under Investigation/Next Steps

- **Optimize the cathode formation with component and compositions**
  - **sulfur**
  - **selenium/selenium compounds**
  - **Robust conductive matrix with carbons/holey graphene**

- **Solid polymer composite electrolytes/solid state electrolytes (SSE)**
  - **Further Ionic conductivity improvement**
  - **SSE/Li metal and SSE/cathode interfacial impedance**

- **Optimization for the design of cathode and solid state electrolyte to maximize the energy density with practical electrode loading, scale up the fabrication, and reduction of production cost need to be addressed in the future development**

- **Leverage the results from our research partners into our project:**
  - **Argonne National Lab (ANL) for S/Se/holey graphene formulation optimization**
  - **Pacific Northwest National Lab (PNNL) for sulfide-based solid-state electrolyte**

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Thank you!

Any Questions?