Overview and Progress of the Advanced Battery Materials Research (BMR) Program

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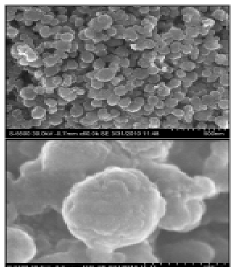
Project ID: ES 108

Outline

- ❑ Advanced Battery Materials Research (BMR)
  - Role
  - Program update
- ❑ Current research emphasis
  - Lithium metal anode and solid electrolytes
  - Sulfur electrode
- ❑ Highlights
- ❑ Summary

BMR Role Within VTO Energy Storage R&D

Advanced Battery Materials Research (BMR Program)

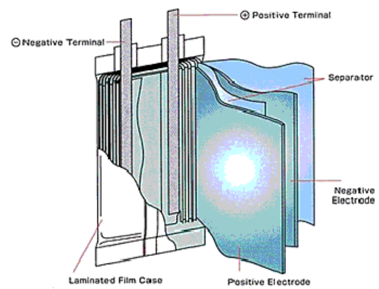


- ❑ High energy cathodes including sulfur
- ❑ Alloy, lithium metal anodes
- ❑ High voltage electrolytes
- ❑ Solid State electrolytes

Cell Materials Targets

- ❑ Anode capacity > 1000 mAh/g
- ❑ Cathode capacity > 300 mAh/g
- ❑ High-voltage cathodes & electrolytes stable up to 5V
- ❑ Solid-polymer electrolytes with $>10^{-3}$ S/cm ionic conductivity

High Energy & High Power Cell R&D (ABR Program)



- ❑ High energy couples
- ❑ High energy and rate electrodes
- ❑ Fabrication of high E cells
- ❑ Cell diagnostics
- ❑ Improved manufacturing processes

Cell Targets

- ❑ 350 Wh/kg
- ❑ 750 Wh/Liter
- ❑ 1,000 cycles
- ❑ 10+ calendar year life

Full System Development & Testing (Developer Program)

USABC UNITED STATES ADVANCED BATTERY CONSORTIUM LLC

- ❑ Focus on cost reduction, life and performance improvement
- ❑ Robust battery cell and module development
- ❑ Testing and analysis
- ❑ Battery design tools

Battery Pack Targets

- ❑ \$125/kWh EV pack cost
- ❑ Fast charge (80% SOC in 15 minutes)
- ❑ \$180 12V start/stop pack cost

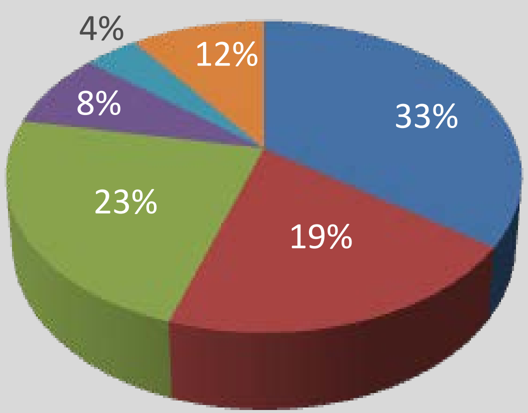
BMR Program (1)

- Previously known as:
  - Batteries for Advanced Transportation Technologies (BATT)
  - Exploratory Technology Research (ETR)
- 10 topic areas, 49 research projects (44 posters)
  - Electrode modeling, diagnostics, cell analysis, silicon anodes, cathodes, metallic lithium & solid electrolytes, sulfur electrodes, lithium air and sodium ion batteries.
  - 3 research projects (on liquid electrolytes) completed in FY 2015 (ANL, Daikin America and Wildcat Inc.)
- Participants include universities, national laboratories, and industry.
- Funding mechanisms:
  - Annual Operating Plan (AOP) process for the national laboratories.
  - Federal Opportunity Announcements (FOAs) for awards to universities and industries.

BMR Program (2)

Budget

FY2016 VTO Energy Storage: $99.4M



Poster Presentations

- 44 posters from BMR

Topic	Posters
Modeling and Diagnostics	14
Alloy Composite Anodes	2
Advanced Cathode Materials	6
Advanced Electrode Architecture	4
Lithium Metal and Solid Electrolytes	6
Sulfur Electrode	9
Air Electrode - Electrolytes	2
Sodium Ion	1

- 22 posters from BES

BMR Program (3)

- Current FOA areas of interest include:
  - Electrolytes and additives, self healing electrolytes; solid and polymer electrolytes, and Li metal protection
  - Diagnostics
  - Modeling
- Proposals are being evaluated and notification of awards will be announced in late summer
- Estimated number of awards 10-12
- Research projects to be started on October 1, 2016

BMR Program (4)

Cathode Workshop, ORNL (March 15, 2016)

Goal: Brainstorm and address current technical challenges related to high voltage lithium-ion cathodes:

1. High voltage redox and anionic stability;
2. Irreversible structural transformation; and
3. Interfacial stability.

Conclusions

- ❑ Continue emphasis on Ni-rich NMC, spinel substituted excess lithium NMC and ensure high voltage stability
- ❑ Stabilize the structure & composition of multi-lithium polyanionic chemistries containing TM's cations at higher oxidation state & address issue of oxygen evolution at V > 4.3 V
- ❑ Cation disorder cathode composition with no voltage fade or hysteresis (e.g., $Li_{1.21}Mo_{0.467}Cr_{0.3}O_2$) and investigate reversible anionic redox activity

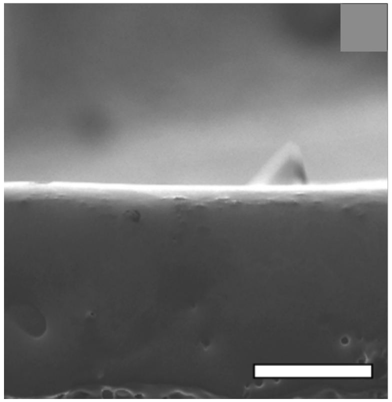
Emphasis: Li Metal Anode

Opportunity

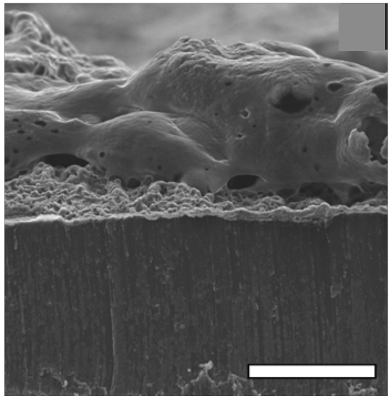
- ❑ Dramatic increases in specific and volumetric energies possible

Objectives

- ❑ Key technical hurdle is to prevent the gradual loss of lithium and impede dendrite formation while providing adequate power
- ❑ This will be addressed through:
  - – Improved understanding of the chemical and physical processes that consume lithium at the electrode-electrolyte interface
  - – Electrolyte additives to prevent dendritic Li growth
  - – Engineered barrier materials, solid or composite electrolytes to stabilize the anode-electrolyte interface



Before cycling (with SEI layer)



10 cycles

Evolution of an SEI Layer on Cycling of a Metallic Lithium Electrode (scale bars represent 100 microns)

Source: ORNL

Emphasis: Solid Electrolytes

Barriers

- ❑ Not all are stable against lithium
- ❑ Have relatively poor ionic conductivity at room temperatures
- ❑ Exhibit inherently very large interfacial impedance
- ❑ Brittle and difficult to fabricate

Approaches

- ❑ Perform mechanical studies through state-of-the-art nano-indentation techniques to probe the surface properties of the solid electrolyte and the changes occurring to lithium
- ❑ Develop composite electrolytes (polymer and ceramic electrolytes) – investigate lithium ion transport at the interface to study the effective ionic conductivity achievable for the composite membrane
- ❑ Identify the relation of defect types that could impact the current density limit in Garnet-based electrolytes
- ❑ Computationally and experimentally study the interfacial structure-impedance relationship in Garnet-based electrolytes to design new materials (U Maryland)

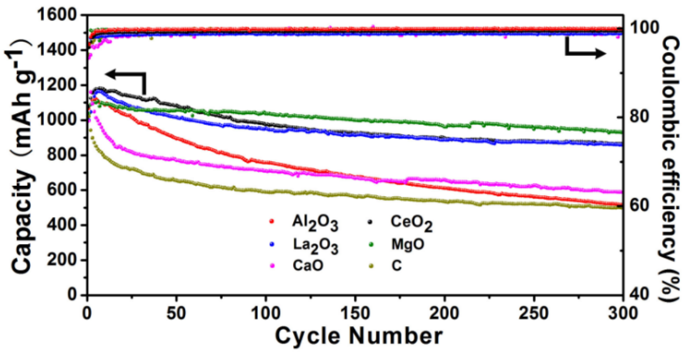
Emphasis: Sulfur Electrode

Barriers

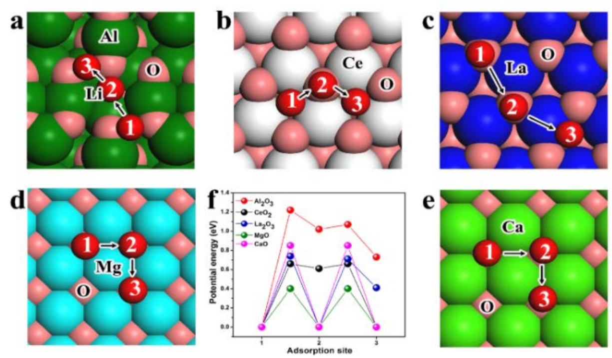
- ❑ Formation/dissolution of polysulfides
- ❑ Sluggish kinetics of subsequent conversion of polysulfides to Li_2S
- ❑ High diffusivity of polysulfides in the electrolyte
- ❑ Insulating nature or poor conductivity of sulfur/Li_2S
- ❑ Volumetric expansion/contraction of sulfur
- ❑ Low mass-loading

Approaches

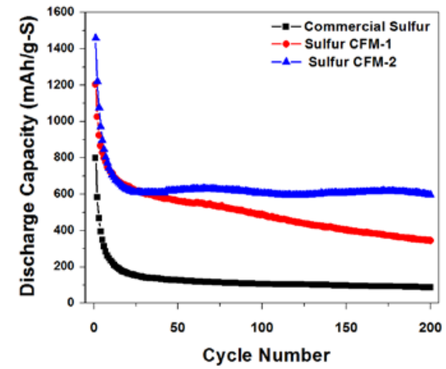
- ❑ Identify basic mechanisms using *in situ*-EPR and NMR studies
- ❑ Explore sulfide, selenide and oxide composite electrodes showing cycling up to 300 cycles
- ❑ Use of lithium-ion conductor coatings and matrices showing low fade rates (<0.003% per cycle)
- ❑ Mesoscale modeling to understand polysulfide mechanisms



Specific capacity improvement by use of oxide composite electrodes upon prolonged 300 charge-discharge cycles at 0.5C

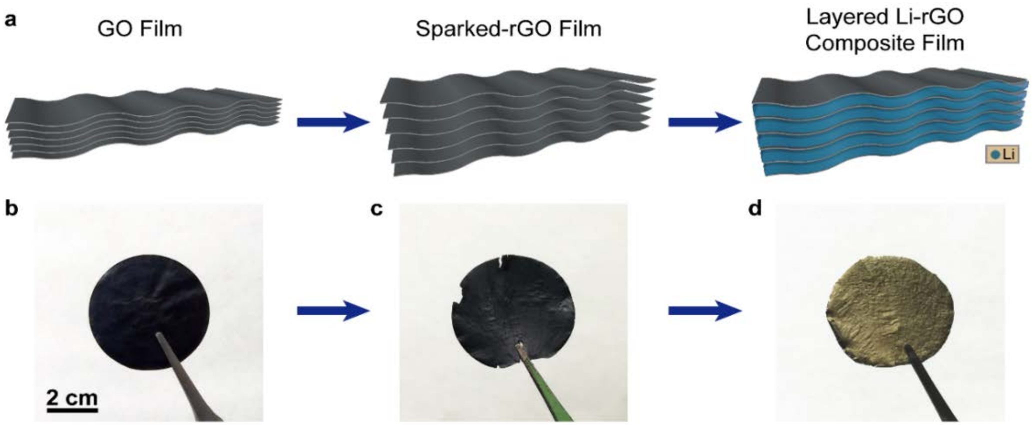


Minimum energy path for lithium ion diffusion on oxide surfaces and Potential energy profiles for Li^+ diffusion along different adsorption sites

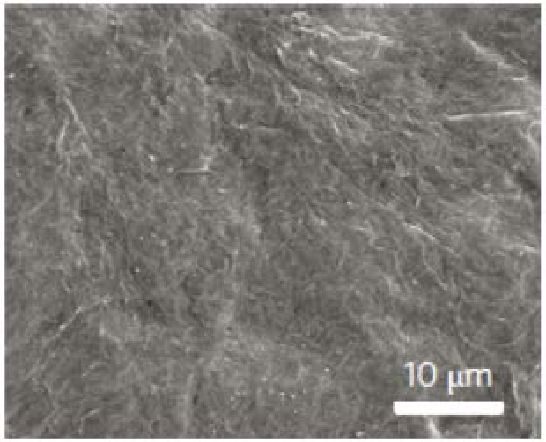


Nanoporous CFM containment and improvement in cycling stability when tested at C/6 rate

Highlight: Layered Reduced Graphene Oxide with Nanoscale Interlayer Gaps as a Stable Host for Li Metal Anodes



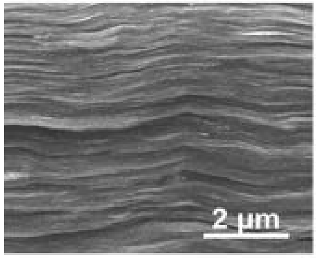
After 10 cycles, the surface is smooth without Li dendrites



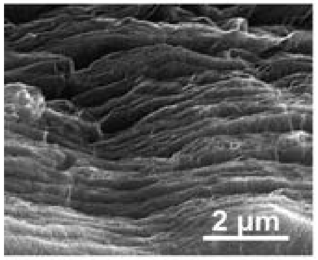
Source: Stanford University

Cross-sectional View

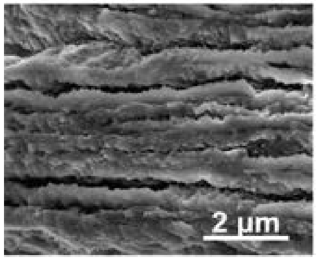
Pristine GO film



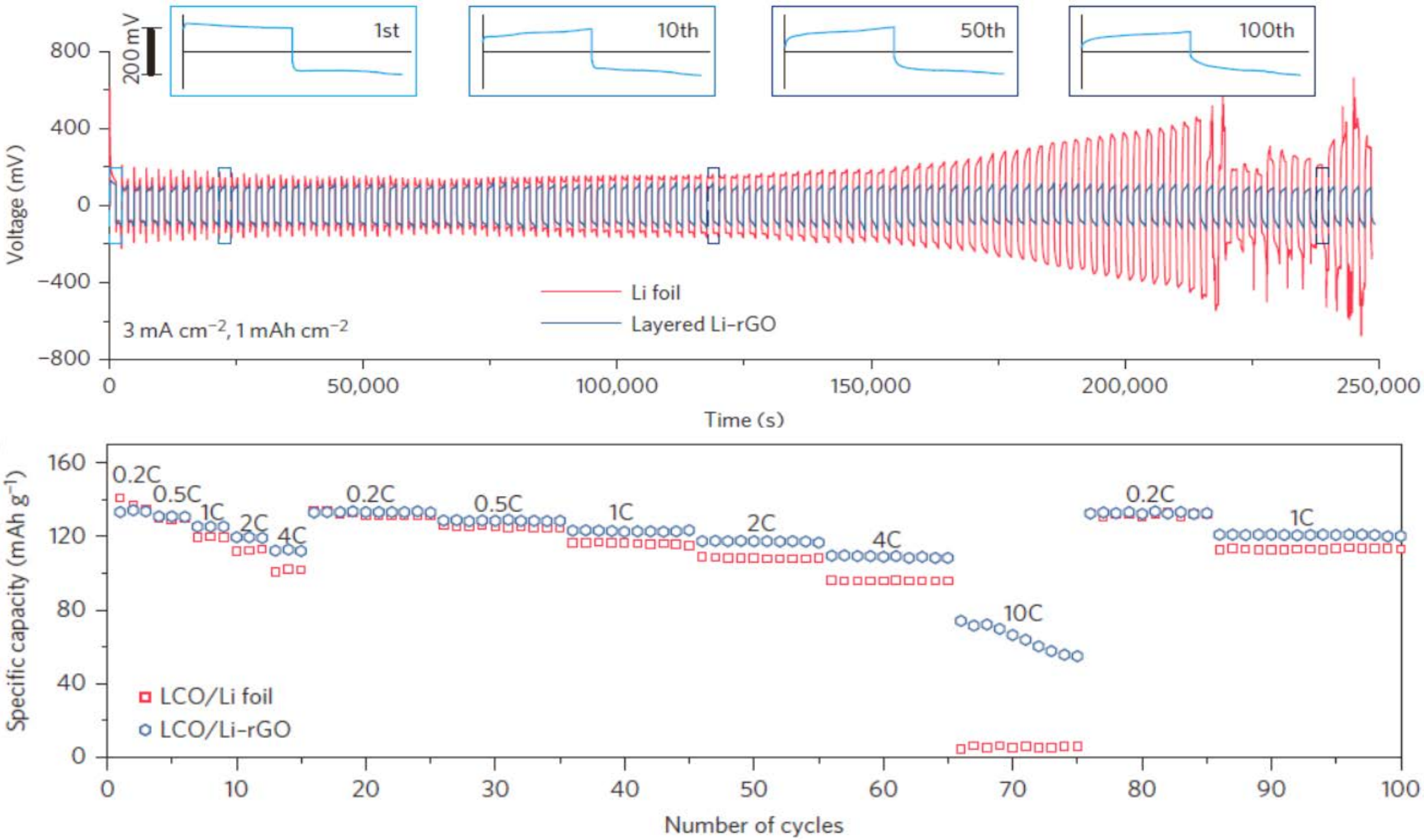
Sparked rGO film



Li-rGO composite



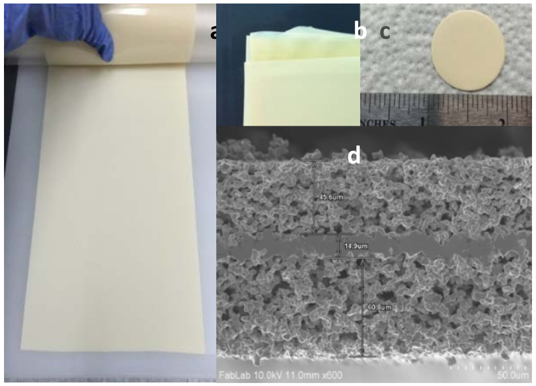
Highlight: Cycling of Li–reduced Graphene Oxide Electrodes



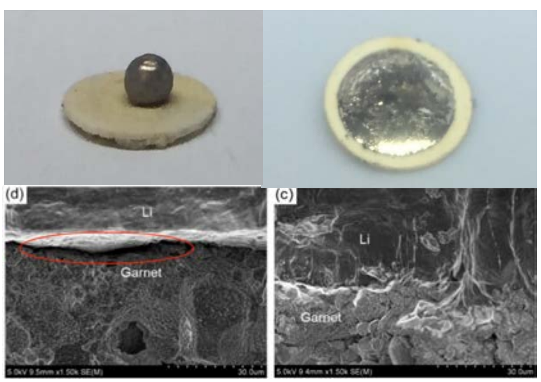
Source: Stanford University

Highlight: Overcoming Interfacial Impedance in Solid-State Batteries

- ❑ Developed scalable and reproducible process to fabricate multilayer garnet structures

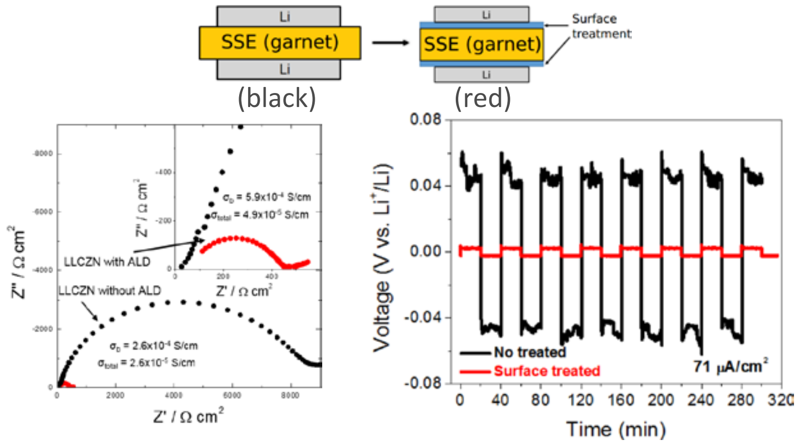


- ❑ Developed surface treatment that allows Li metal to wet garnet surface

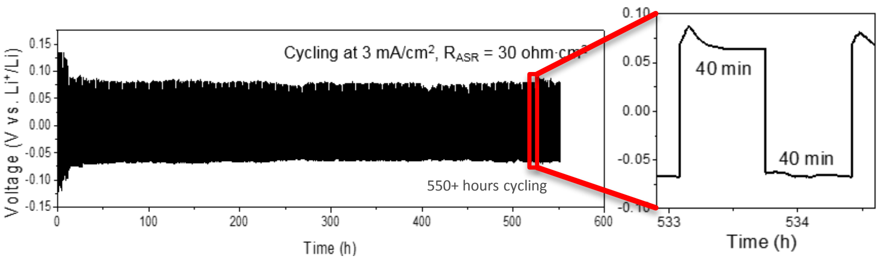


Source: University of Maryland

- ❑ Surface treatment dramatically reduces interfacial resistance

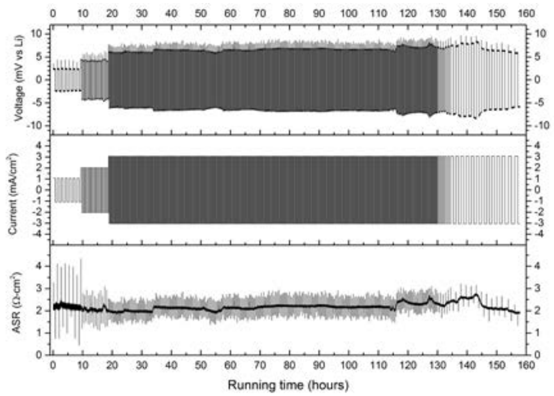


- ❑ Long term, high rate lithium cycling with no degradation
  - – Demonstrated in multiple cells with planar, bilayer and trilayer configuration
  - – Demonstrated reduction in overpotential due to negligible interfacial impedance

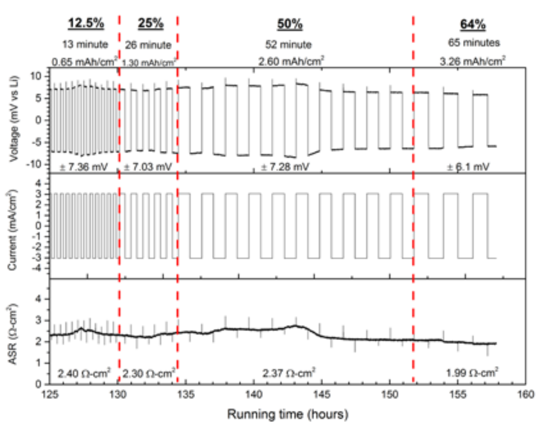


Highlight: Overcoming Interfacial Impedance in Solid-state Batteries

- ❑ Demonstrated high current density 3 mA/cm^2

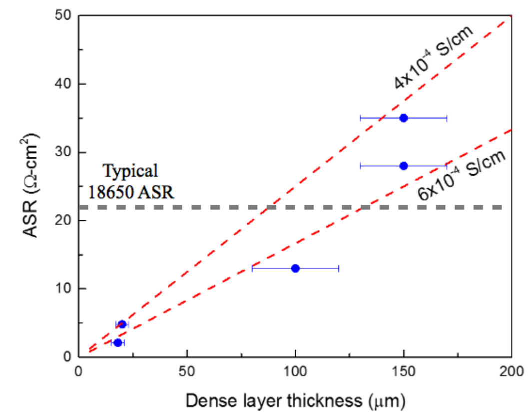


- ❑ …and high Li capacity (3.26 mAh/cm^2) cycling in trilayer garnet with no degradation or shorting

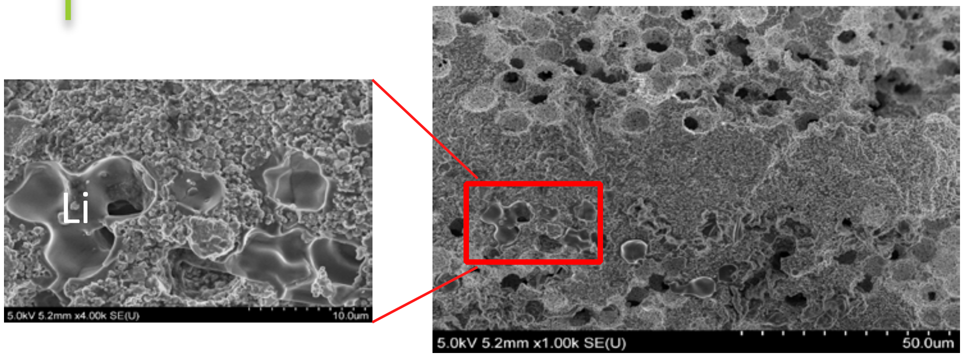


Source: University of Maryland

- ❑ …with extremely low ASR (2 Ωcm^2)



- ❑ …and demonstration of Li metal filling garnet pores



Summary

- ❑ Advanced Battery Materials Research (BMR) Program underwent a recent name change
  - Previously known as BATT, ETR
  - Name better reflects the materials focus of the program
  - 10 Topic areas
  - 49 Research projects
  - The new website is: http://bmr.lbl.gov
- ❑ Continue to closely coordinate with BES (JCSER), ARPA-E and Office of Electricity

Cathode Workshop, ORNL (March 15, 2016)