Solid-state Architecture Batteries for Enhanced Rechargeability and Safety (SABERS)

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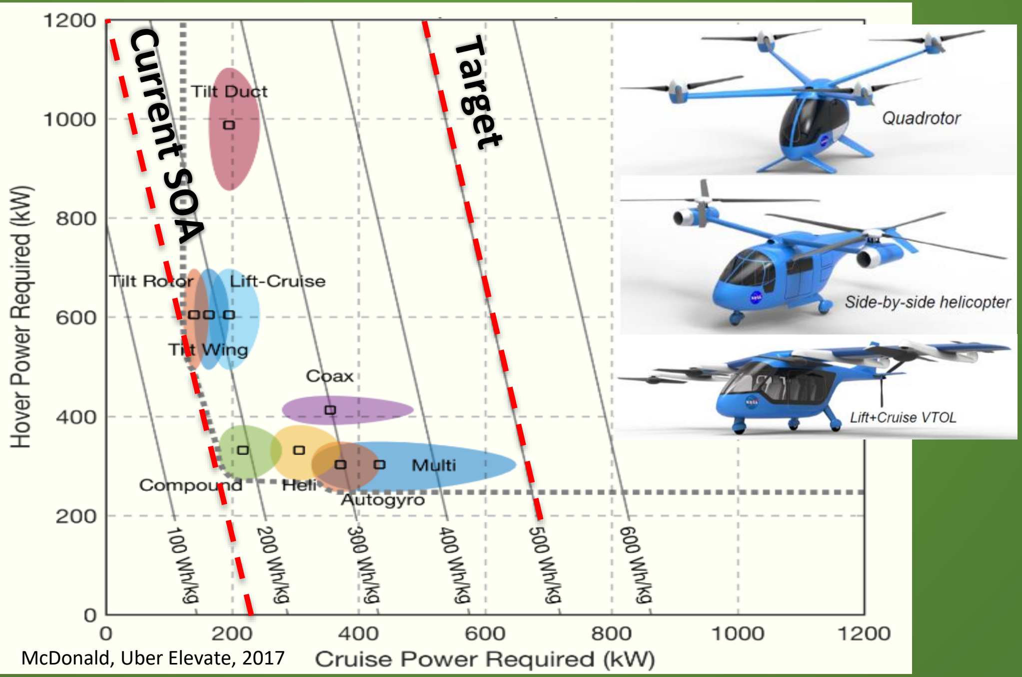
The Problem

Current SOA batteries are not designed to meet the unique performance & safety requirements of electric aircraft

Battery Performance Requirements

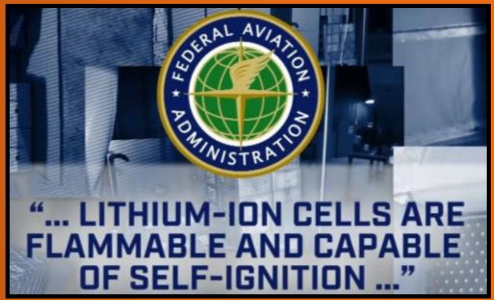
- NASA Battery Workshop 2017 and industry representatives state "The primary barrier to electric aviation is battery performance"
- SOA lithium ion batteries do not meet energy density requirements needed to enable electric aircraft designs
- Unique flight critical metrics (e.g. high power) required



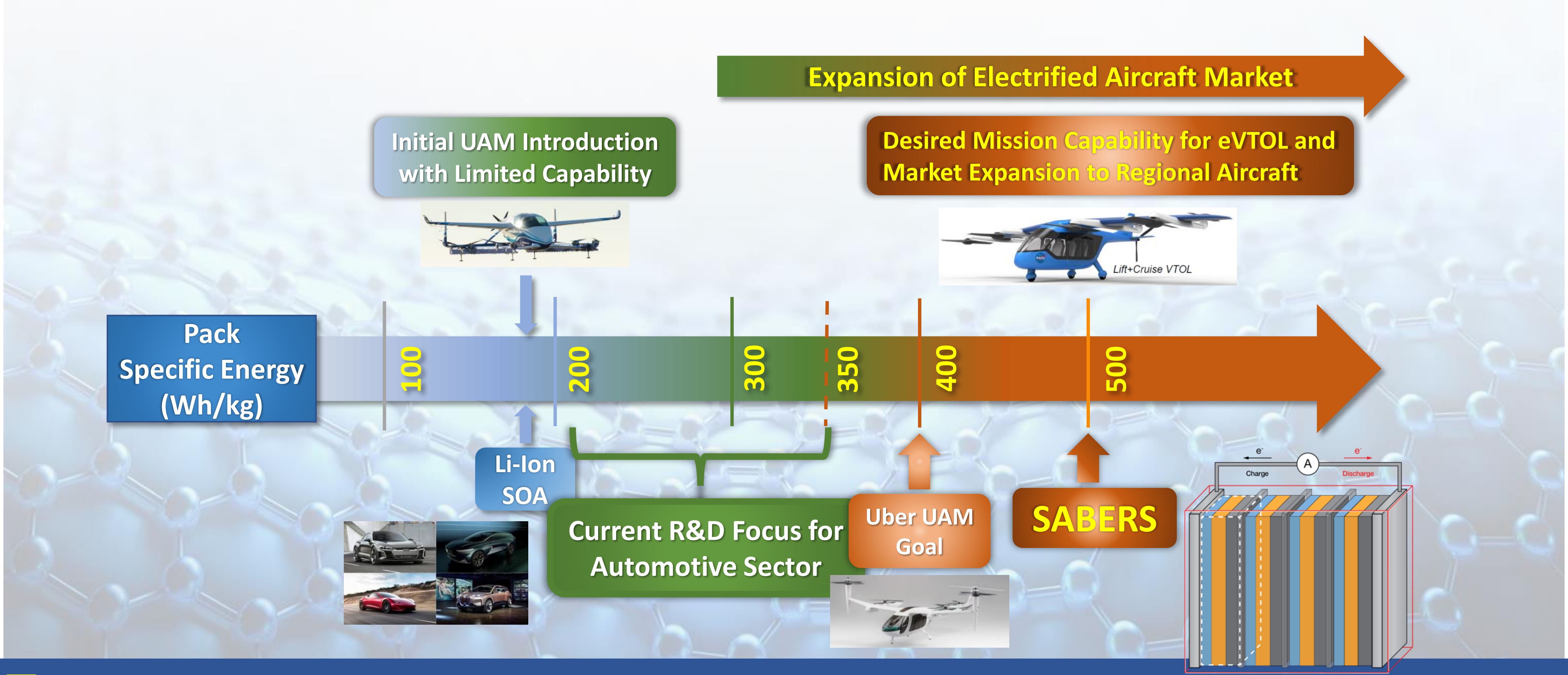
Vehicle Performance & Efficiency

Battery Safety Requirements

- Current batteries under development will always have fire safety challenges due to flammable electrolytes used
- Safety is required for aerospace applications
- SOA lithium ion batteries have caused a number of safety incidents on aircraft
- Parasitic weight from excess packaging and cooling is undesirable



SABERS Focused on Electric Aircraft



- ❑ Current performance targets for the automotive sector are a battery pack with 250 – 300 Wh/kg

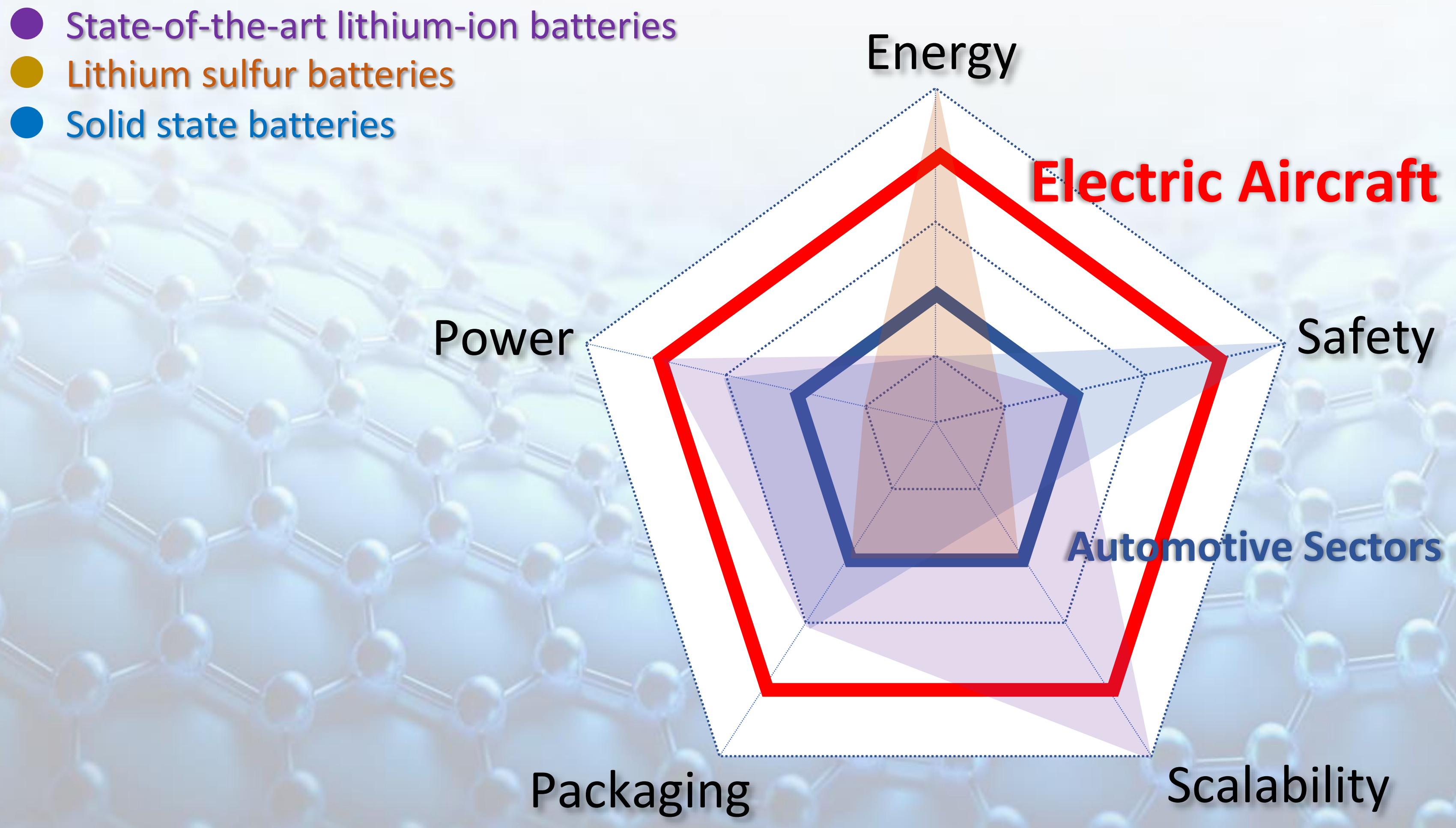
Aeronautics Challenges

- Can a battery be designed for electric aircraft, following system level analyses, that provides the combination of required properties?
  - Safety
  - Energy density
  - Discharge rate
  - Packaging design for minimal weight
  - Scalability

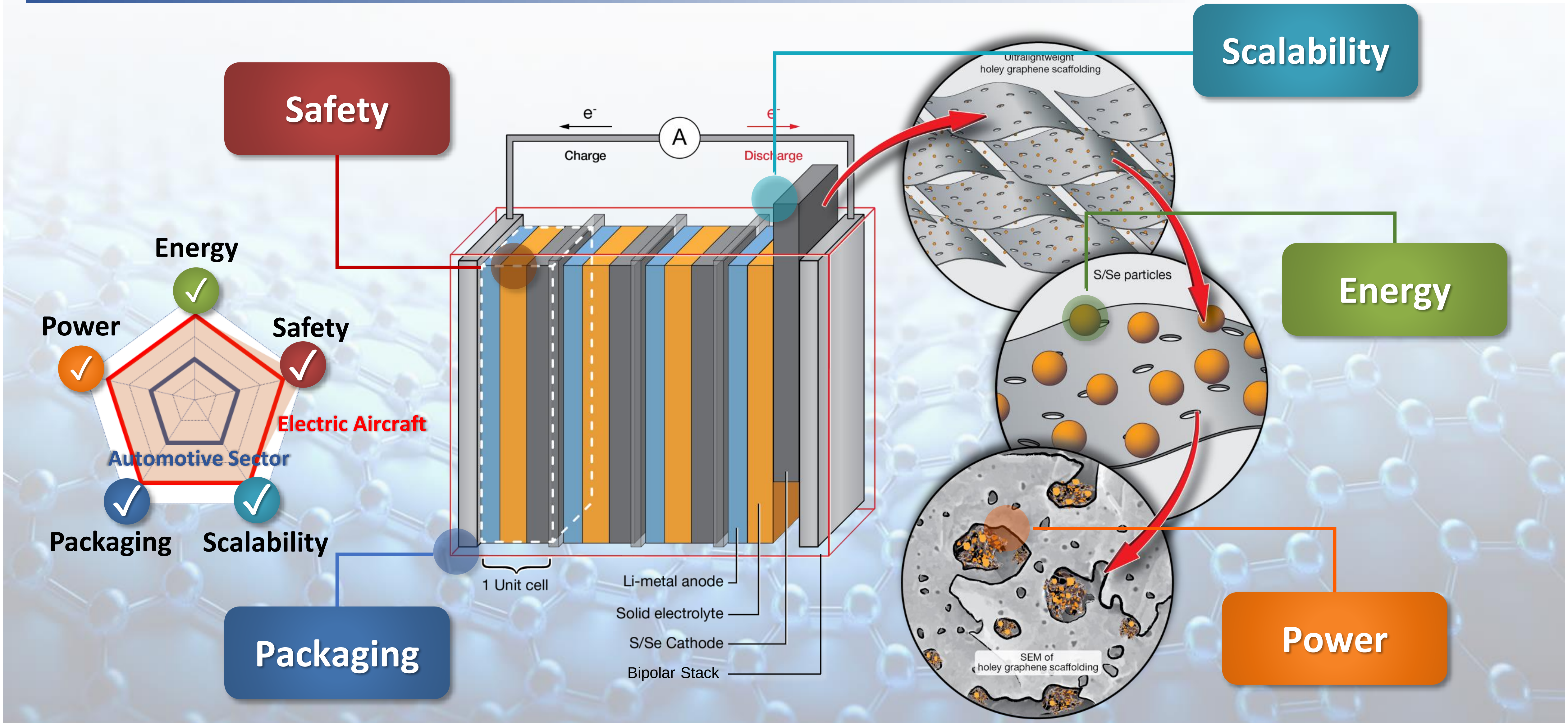
SABERS Concept: Design a battery using system level analyses to guide target properties, combine existing materials technologies, and a bi-polar stack design.

The Big Question

How do we meet ***ALL*** demanding battery needs of electric aircraft?



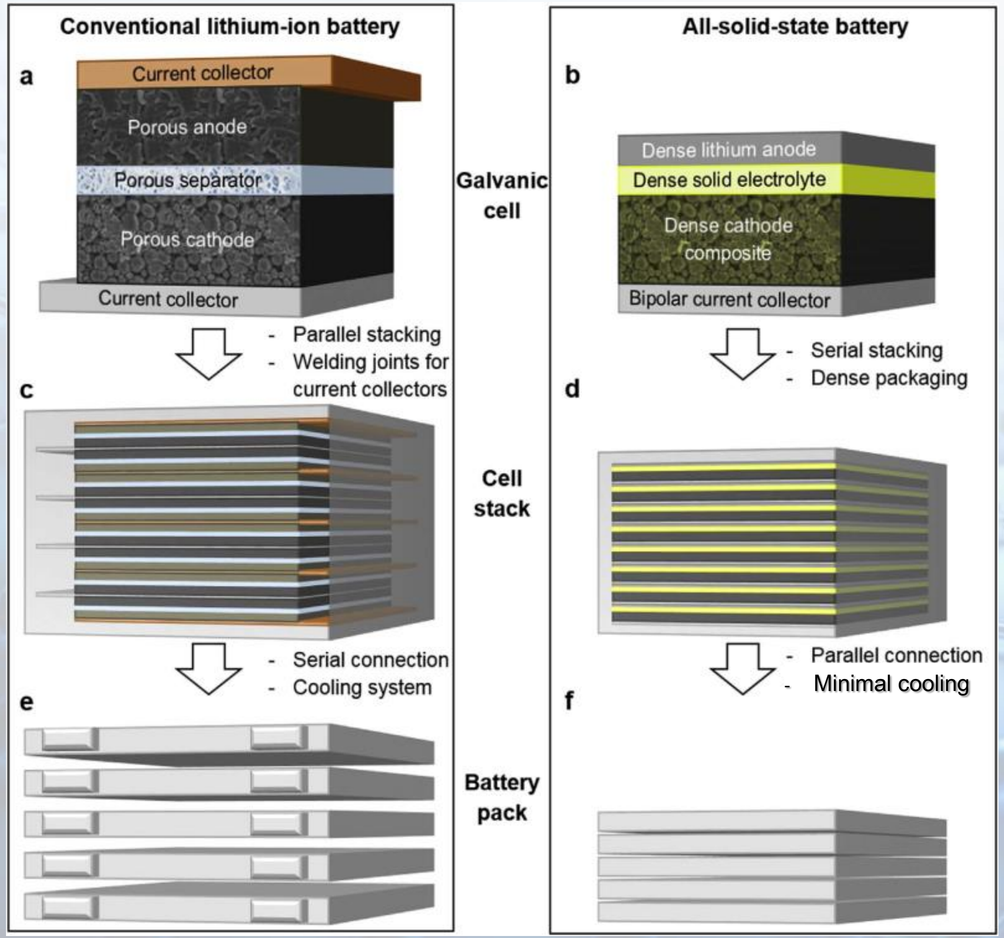
SABERS Transformative Technology



Combination of unique materials technologies to achieve performance goals

Bi-Polar Stack Solid-State Battery

SSE-enabled bi-polar stack design minimizes safety containment in packaging



Lithium-Ion Battery (SOA) Packaging

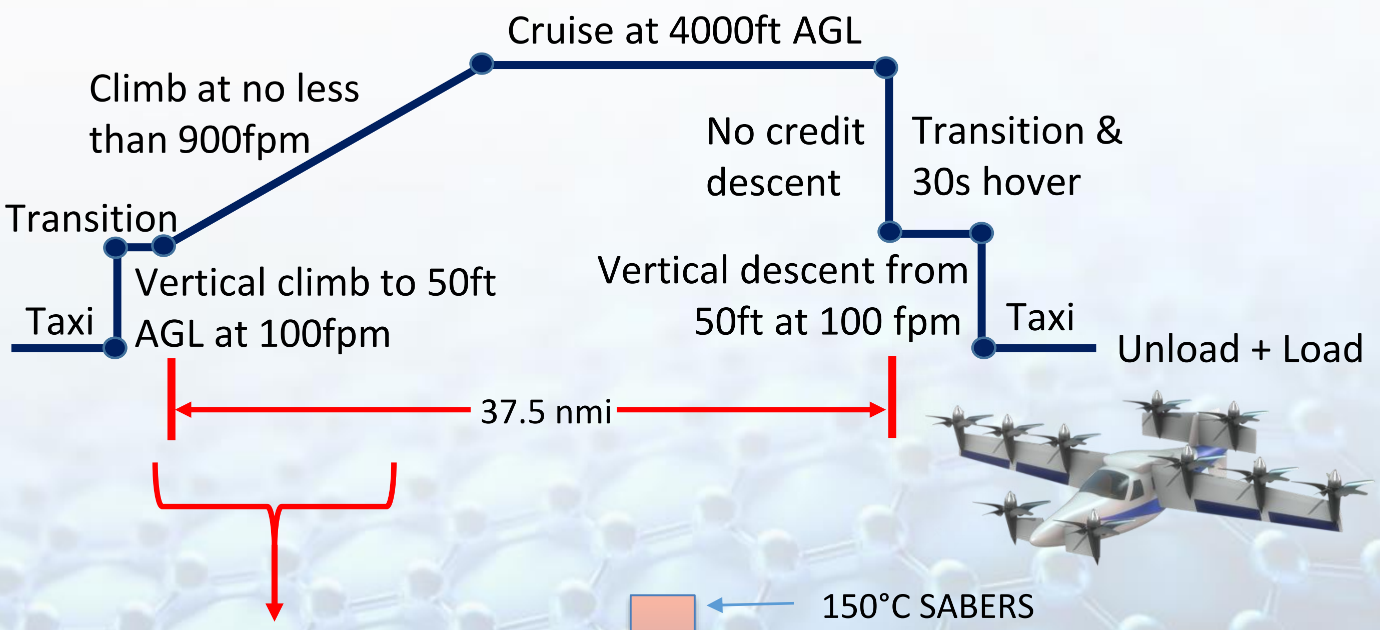
- Contains flammable electrolytes
- Requires heavy housing and cooling system
- The added pack weight reduces energy density

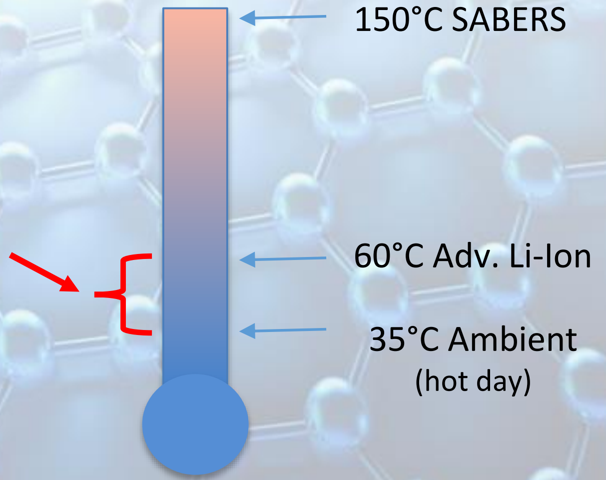
Bi-Polar Stack Packaging Enabled by SSE

- Contains no flammable liquids
- Enables a shared current collector (bi-polar)
- Reduces safety containment weight
- Minimal/passive cooling system possible
- Potential for higher power density and C-rates
- 90% of cell specific energy can be retained in pack

Thermal/Weight Systems Level Analysis

- **SABERS operating temperature (150°C) versus for Li-Ion chemistries (50-60°C)**
- **Thermal heat load well within SABERS temperature limits (simple passive system)**
- **Advanced Li-Ion batteries require:**
  - *Active system*: adds 20-30% weight, 30-50% volume, 1-3% of power used
  - *Semi-passive:* system with phase change material: 10-20% weight and volume penalty



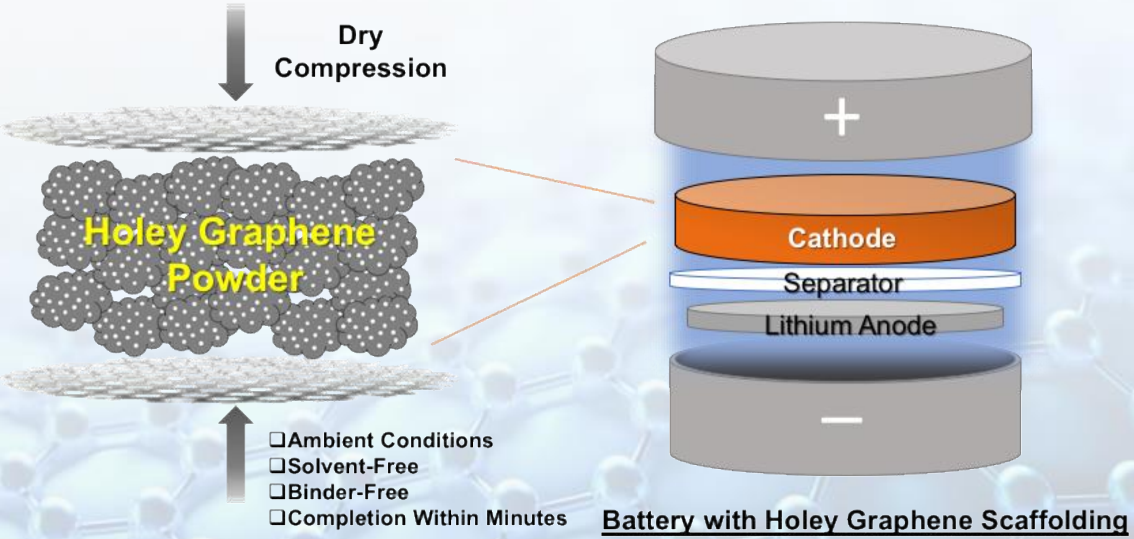


SABERS Bi-Polar Stack

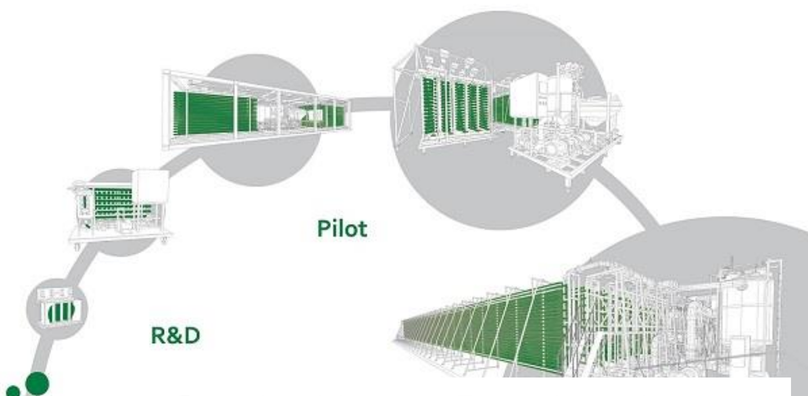
- Effectively 10-30% less battery pack "overhead"
- Improved specific energy and power
- Critical enabling technology for all-electric, battery vehicles/missions

Holey Graphene Conductive Scaffold

<u>Encapsulate S/Se with holey graphene hosts to maximize energy and power utilization</u>

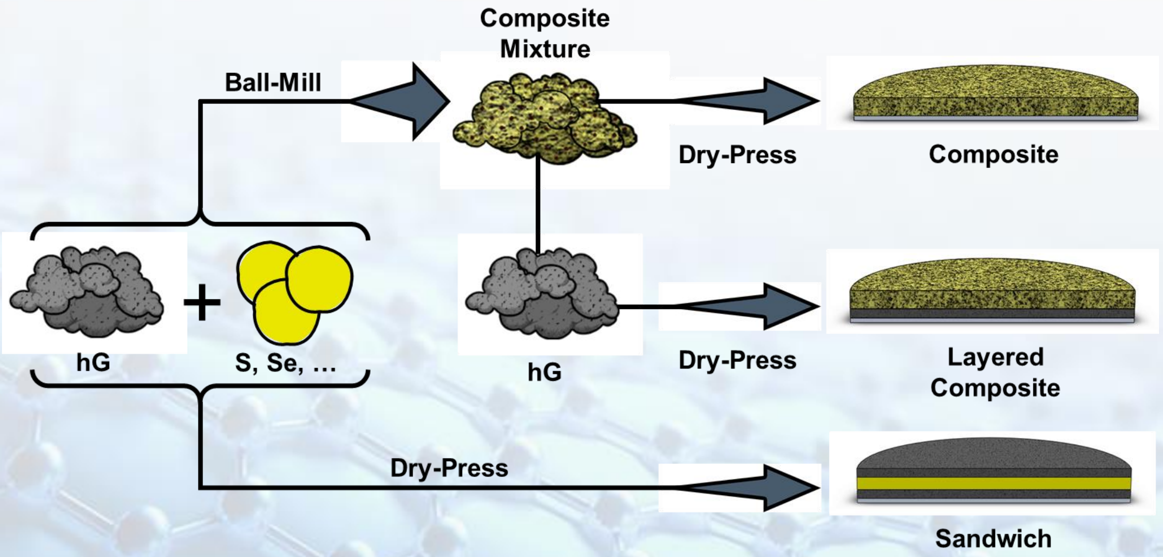


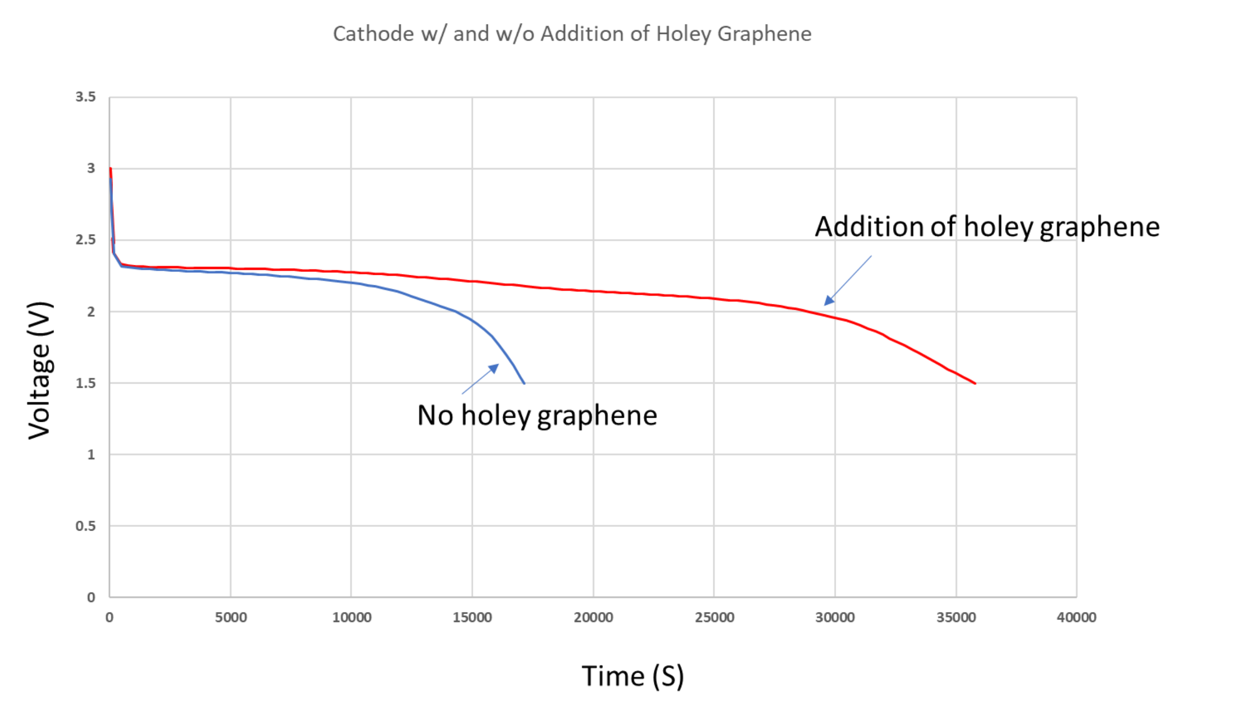
- ❑ Unique NASA-developed technology
  - ➢ High conductivity, ultralightweight electrode scaffold
  - ➢ Through-thickness ion transport enabling fast kinetics
  - ➢ Enables universal dry electrode processing
  - ➢ Scalable



Scale-Up to Production

Holey Graphene Fabrication and Performance



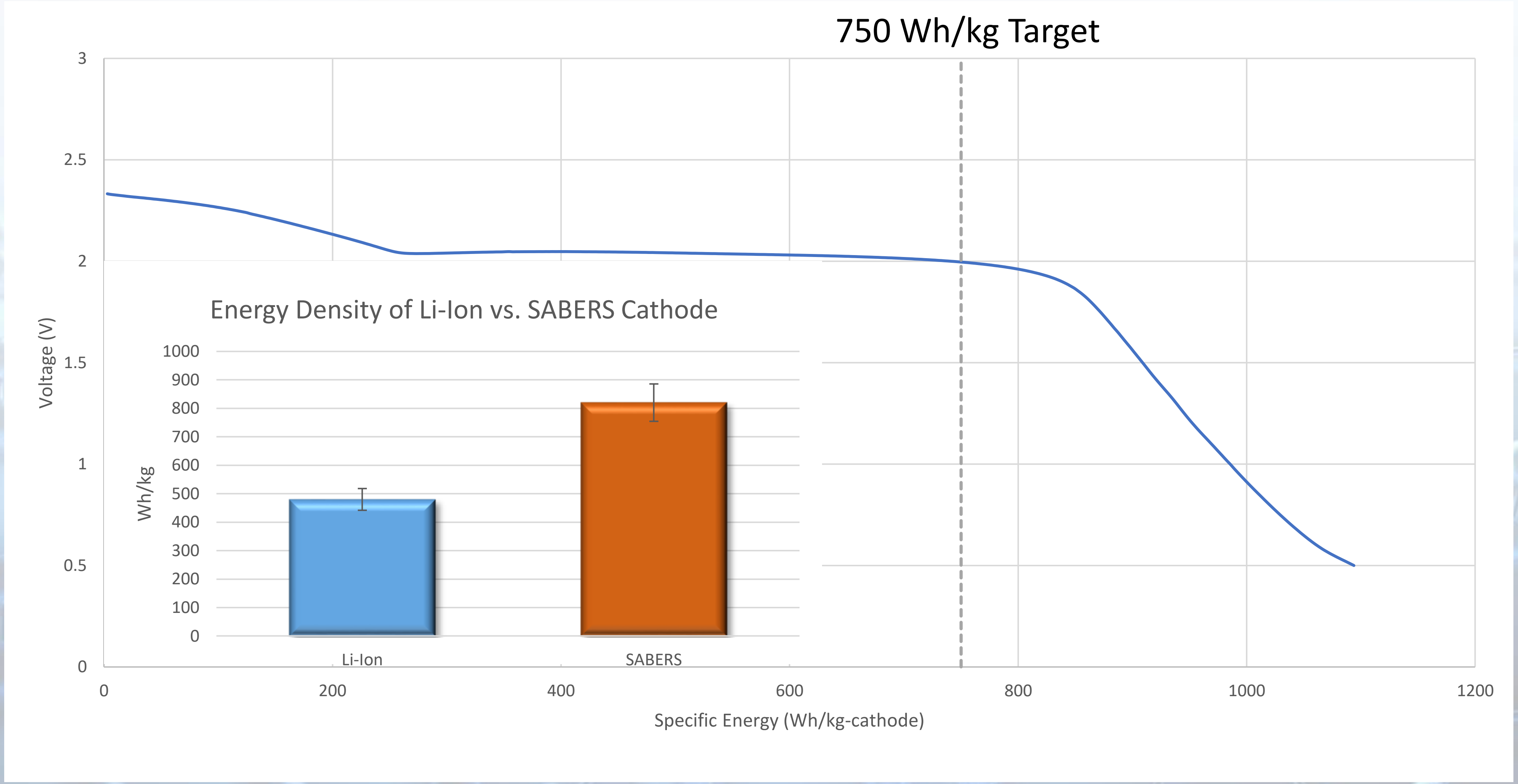


- ❑ High active material content (up to 90 wt%)
- ❑ High mass loading: high areal capacity
- ❑ Excellent current collector– cathode contact

- ❑ **Extremely facile: single-step, no mixing needed**
- ❑ **Widely applicable: S, Se, Se_xS_y, Li_2S**

- ❑ Ultrahigh mass loading (>10 mg/cm^2) cathodes from hG-enabled dry-press technique are advantageous toward cell- and pack-level performance.
- ❑ Addition of holey graphene significantly improves the initial discharge capacity of the cell

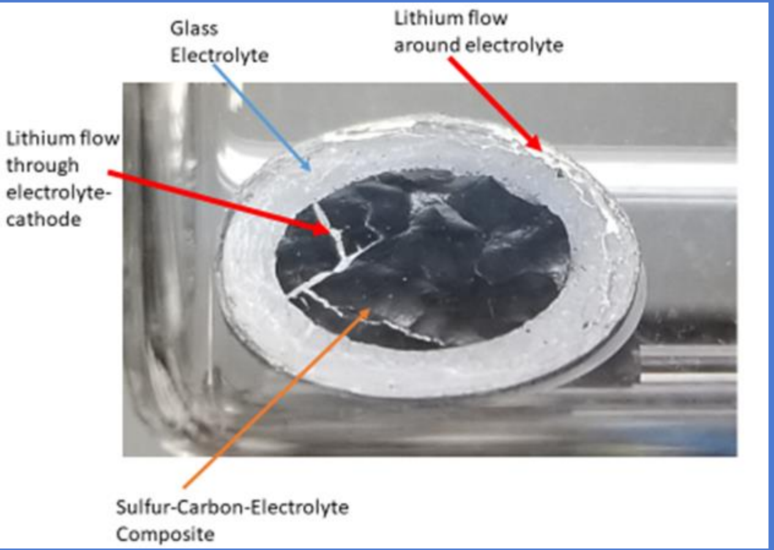
A 0.4C Discharge Rate Exceeds 1100 Wh/kg for thicker electrode (2.8mAhcm^{-2})

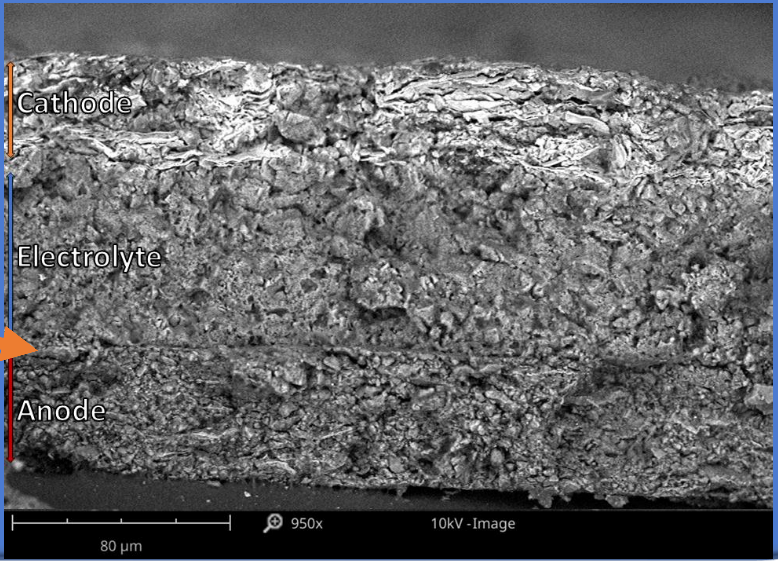


- 50 wt% Sulfur:Carbon with a liquid electrolyte able to achieve 1100 Wh/kg at 0.4C discharge rate

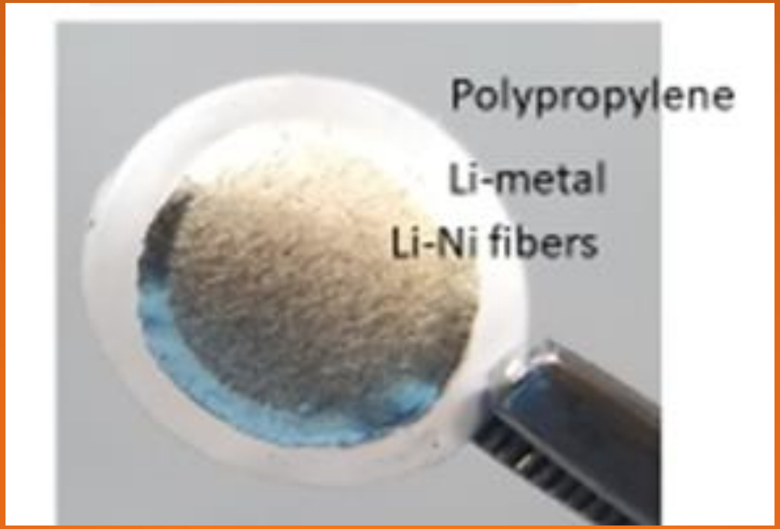
Traditional SSB Manufacturing Approach vs. SABERS Approach

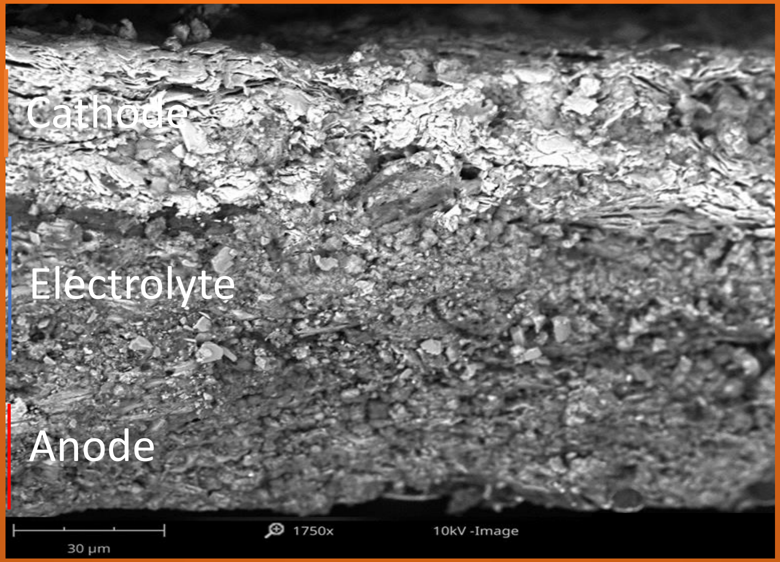
Traditional SSB Manufacturing Approach





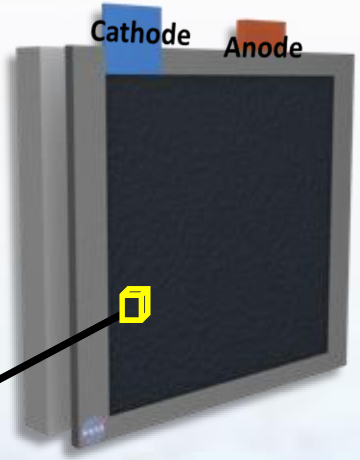
SABERS Approach





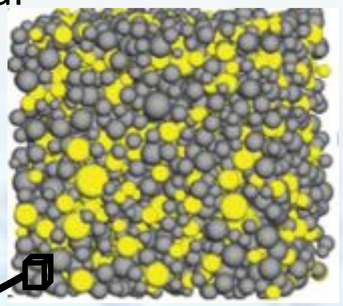
Multiscale Modeling Approach

Battery



- Physics based continuum scale modeling: electrochemical and thermal models
- Experimental benchmarking

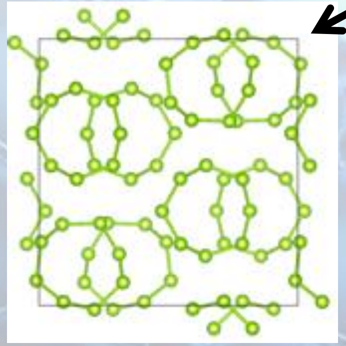
Cathode material



~ 10 – 100 μm

- Particle dynamics methods: electro-mechanical model
- Grain structure properties
- SE/CAM ratios, cathode utilization

Crystal lattice



~ 1 – 2 nm

- Ab initio simulations
- Material and transport properties
- Doping strategies

Computational simplicity

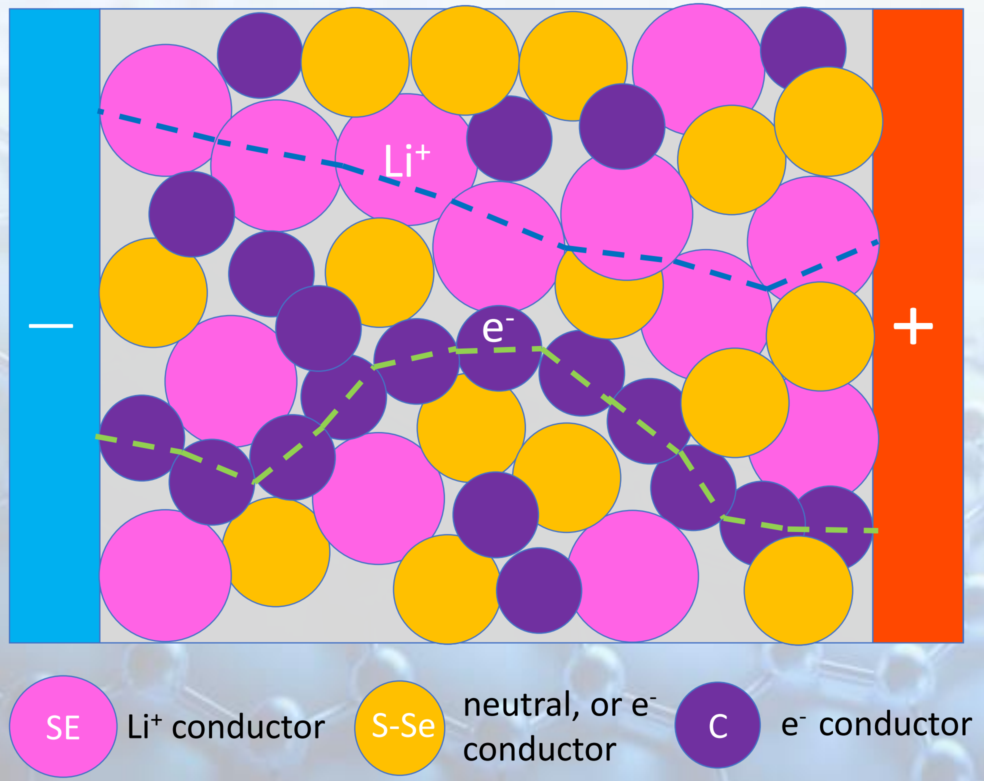
Length Scale

Particle Dynamics Method

Electro-mechanical model: Solid Electrolyte Sphere Approximation Model (SESAM)

(NTR: LAR-19842-1)

Cathode Representative Volume Element (RVE)



- Represents the cathode composite as a system of tightly packed spheres of different types and sizes with assigned specific Li^+ and e^- conductivities.
- Calculates the total conductivities for Li^+ and e^- of the mixed powder composite as dependent on the particle size, density and composition ratio.

*Solid Electrolyte Sphere Approximation Model (SESAM) is pending NASA Release

Particle Dynamics Method

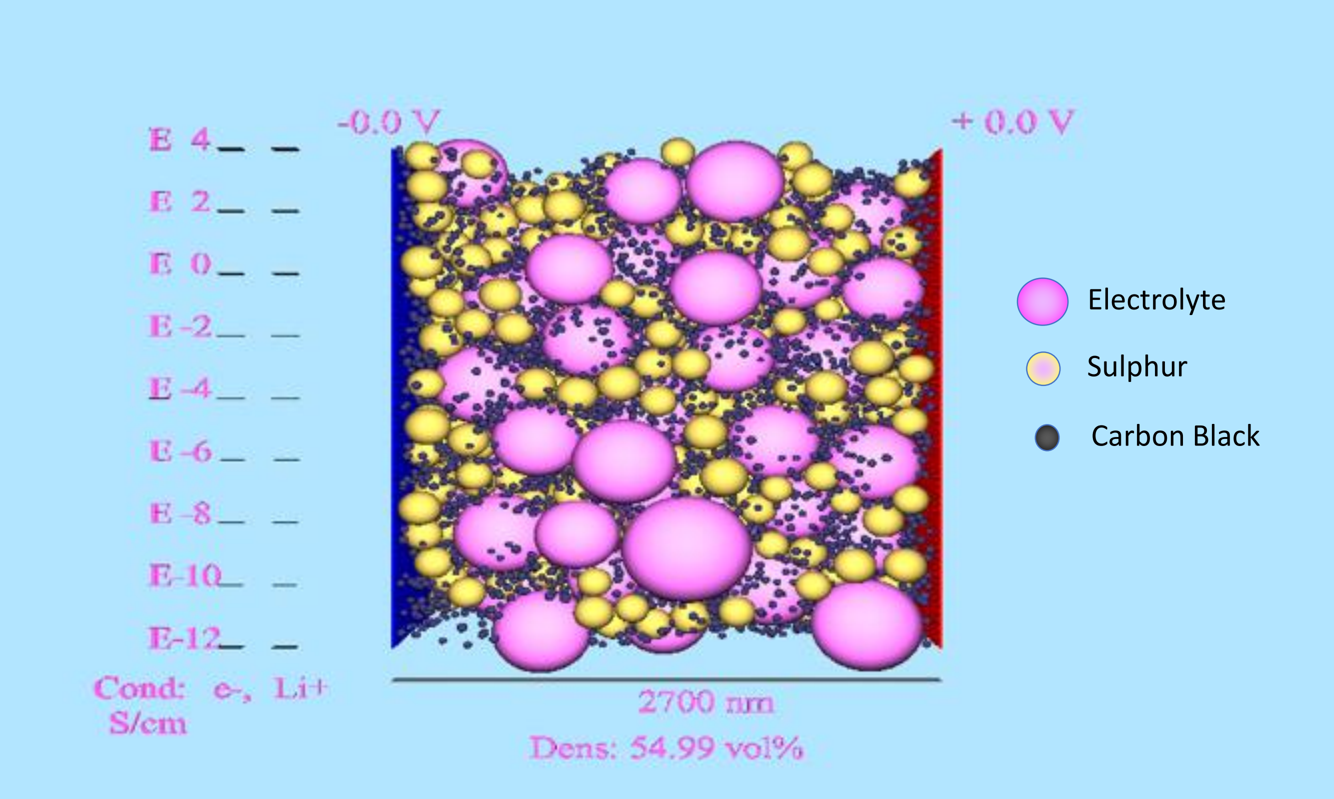
Electro-mechanical model: Solid Electrolyte Sphere Approximation Model (SESAM)

(NTR: LAR-19842-1)

Model construction:

- **Generate particles of given type (SE, C, S) and given size distribution**
- **Fills the system box (or RVE) with particles of all types randomly**

Cathode Representative Volume Element (RVE)



Particle Dynamics Method

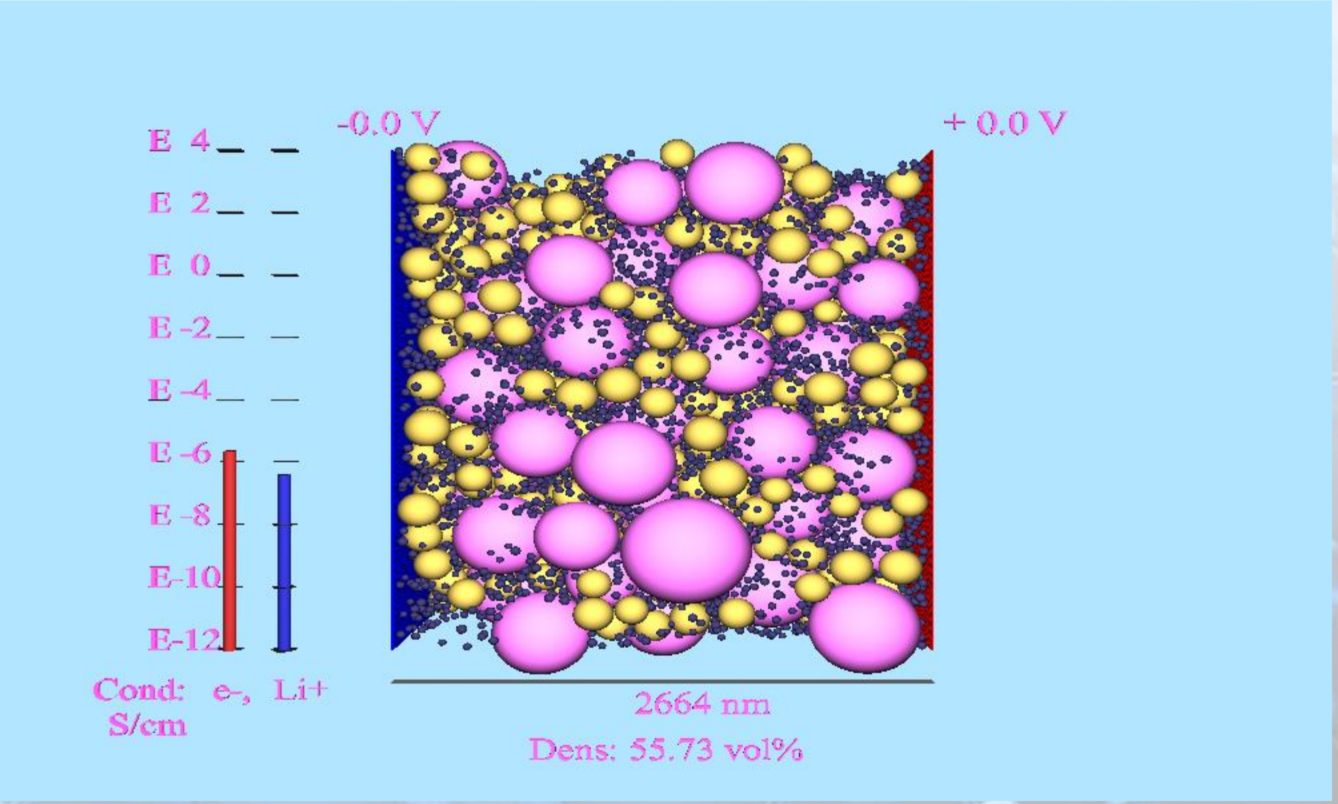
Electro-mechanical model: Solid Electrolyte Sphere Approximation Model (SESAM)

(NTR: LAR-19842-1)

Model construction:

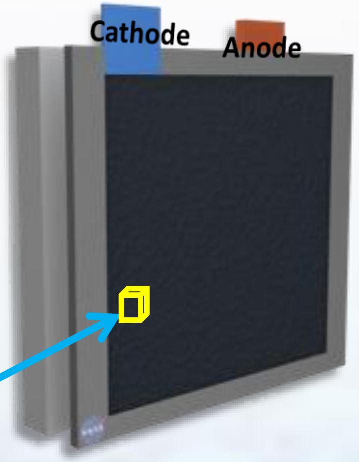
- ❑ Generate particles of given type (SE, C, S) and given size distribution
- ❑ Fills the system box (or RVE) with particles of all types randomly
- ❑ Compress the powder composite

Cathode Representative Volume Element (RVE)



Multiscale Modeling Approach

Computational simplicity



- Continuum Scale
- Physics based modeling
- Experimental benchmarking

Mass conservation

$$\phi \frac{dC_{Li}}{dt} - \frac{\partial}{\partial x}\left(\tilde{\phi} D_{Li}\frac{dC_{Li}}{dx} + uC_{Li}F\frac{d\varphi_2}{dx}\right) = -a\, j_n$$

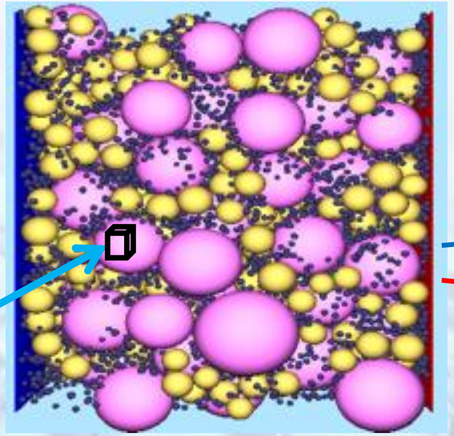
Electron charge conservation

$$\frac{\partial}{\partial x}(i_1) = \frac{\partial}{\partial x}\left(-\sigma\frac{\partial \varphi_1}{\partial x}\right) = a\, j_n F$$

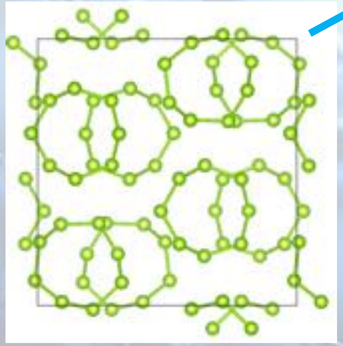
Ion charge conservation

$$\frac{\partial}{\partial x}(i_2) = \frac{\partial}{\partial x}\left(-\kappa\frac{\partial \varphi_2}{\partial x}\right) = - a\, j_n F$$

- Particle dynamics level
- Electromechanical and grain interaction model



$\sim 1 - 10\mu m$



$\sim 1 - 2$ nm

- Ab initio simulations
- Material and transport properties
- Doping strategies

- ❑ SESAM takes input from experimental data and ab-initio QM simulations on material properties
- ❑ SESAM predicts cathode ion and electron conductivities as input to mesoscale battery models

Conclusions

- **Elevated temperature operation is a design parameter that can modified**
  - *If you increase operating temperature from 40 to 50 °C, energy is increased by 10%*
  - ➢ SABERS is a solid-state battery which enables high temperature operation (150 °C)

- **Addition holey graphene improves cathode performance**
  - *Holey graphene provides high electrical conductivity and binderless dry compressibility*
  - ➢ It increases cathode electrical conductivity and initial voltage discharge profile

- **SABERS 1C-rate for lithium-sulfur (804 Wh/kg) is comparable to a 3C-rate for lithium-ion**
  - *The standards for electric aircraft are given in terms of lithium-ion batteries*
  - ➢ Different chemistries require defining unique standards

- **Optimizing the composition ratio between SE, active material, and conductive agent can significantly improve battery performance**
  - *Particle size has a significant effect on the ionic and electronic conductance*
  - ➢ The model suggests using large particles

SABERS Team/Acknowledgements

Aerospace Industry

Aurora FLIGHT SCIENCES A BOEING COMPANY

BOEING

Electrified aircraft is a core NASA thrust

Excitement to partner with world leader in aeronautics technology

Battery Industry

ionic MATERIALS

NASA

Department of Energy

DEPARTMENT OF ENERGY UNITED STATES OF AMERICA

Argonne NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

- NASA is a "thought leader" in aeronautics
- Industry peers state NASA should lead feasibility assessment of 500 Wh/kg battery