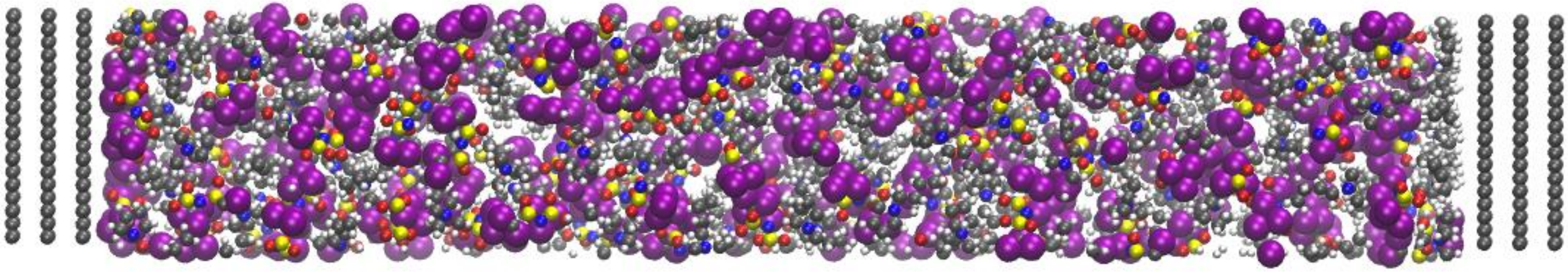


ICME for NASA Aerospace Applications: Batteries for Electric Aviation

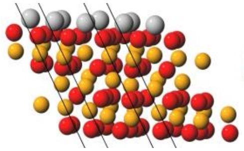
John Lawson
NASA Ames Research Center

ICME for NASA Aerospace Applications

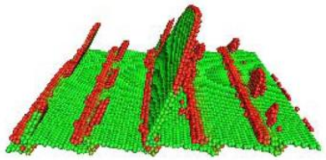
Materials Science: Design "The" Material

Engineering: Design "With" Material

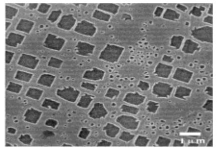
NASA Computational Capability



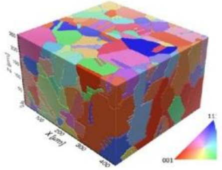
Quantum



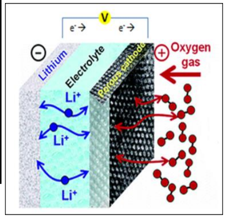
Atomistic



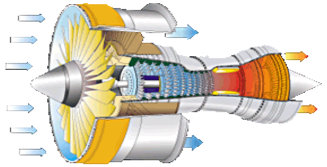
Mesoscale



Continuum



Part



Assembly

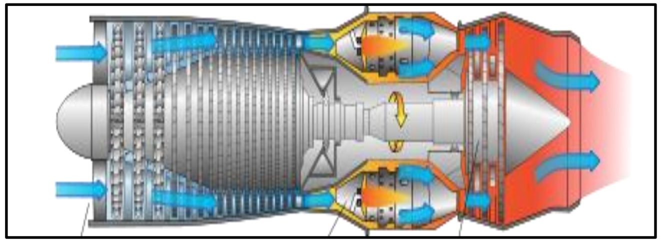
Vehicle

Bring *materials* into the *design cycle* -- Boeing's "*atoms to airplanes*" program

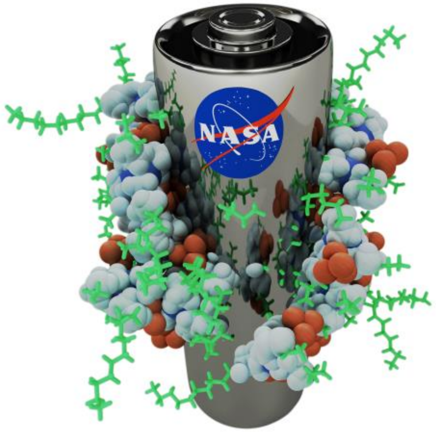
NASA Vision 2040

NASA Vision 2040 Goal: Enable the rapid, low cost design, development, certification and deployment of application specific advanced aerospace materials

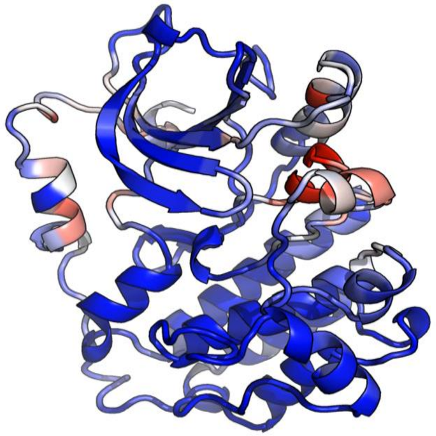
NASA Ames Computational Materials



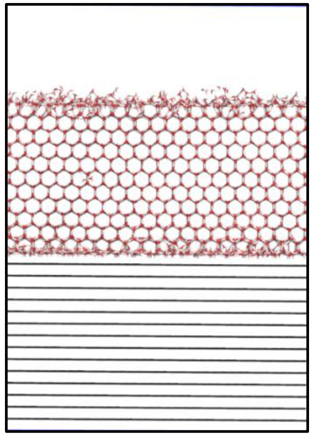
Metals



Batteries



Biosciences



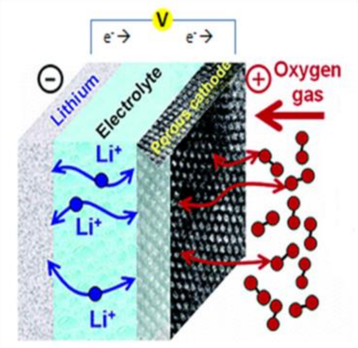
Anti-Icing Coatings

NASA Strategic Plan for Green Aviation

Strategic Thrust 4:
Transition to Alternative Propulsion and Energy

Alternate Propulsion Demonstrators

Li-Air Battery



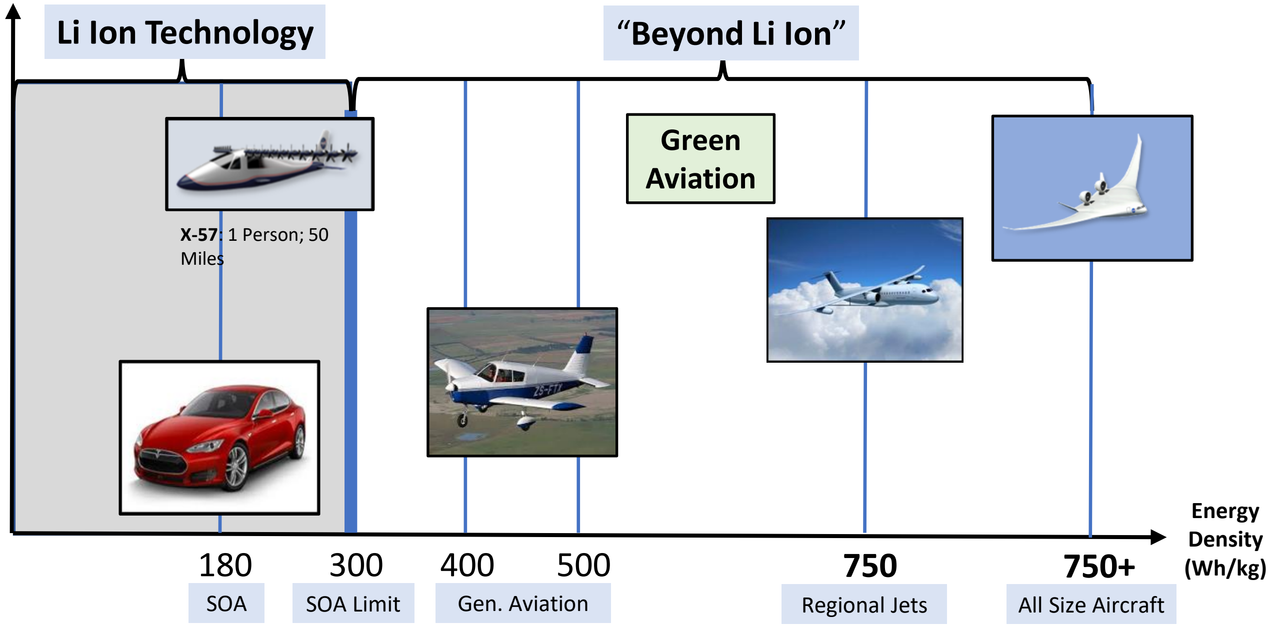
- Zero emissions
- Low noise
- Energy efficient

Batteries are a critical enabler for electric aircraft

Green Aviation Battery Requirements

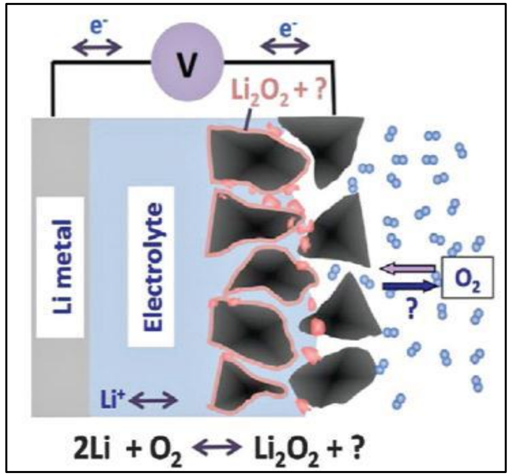
Major requirement is: High Energy Density

Other requirements are **rechargeable**, **safety**, power, recharge time, cost, etc.

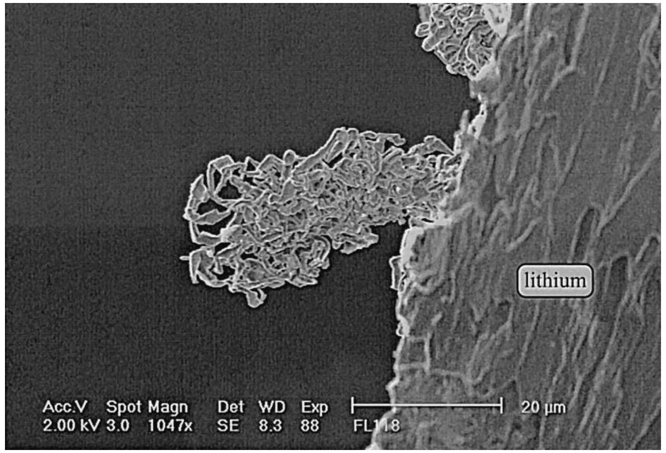


Electric aircraft have the most extreme requirements of any battery application

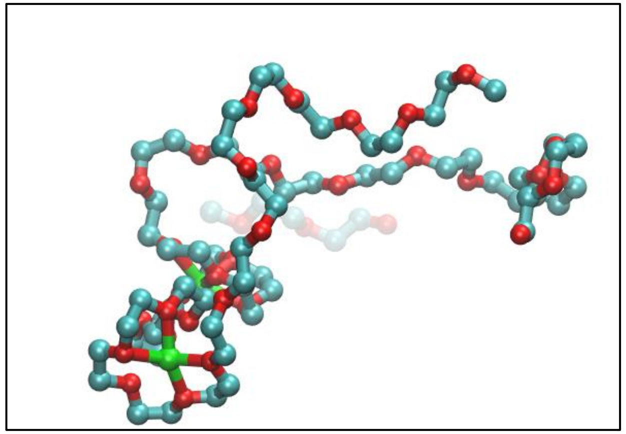
Energy Storage Research at NASA Ames



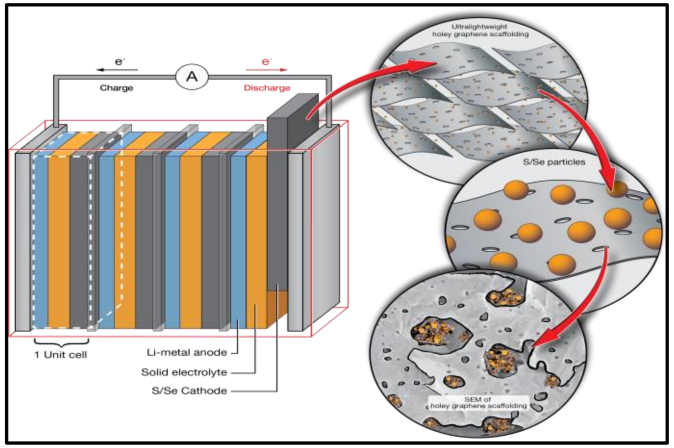
Li-Air Batteries (LiON)



Ionic Liquid Electrolytes for Li Metal

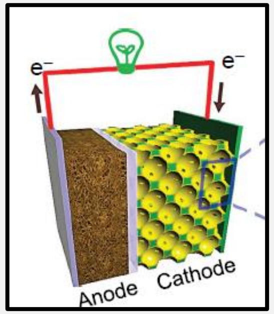


Polymer Structural Electrolytes

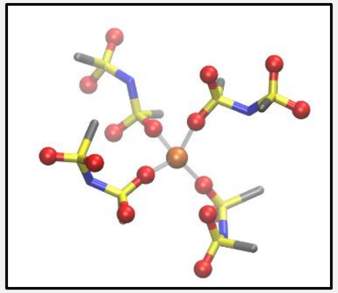


All Solid-State Batteries (SABERS)

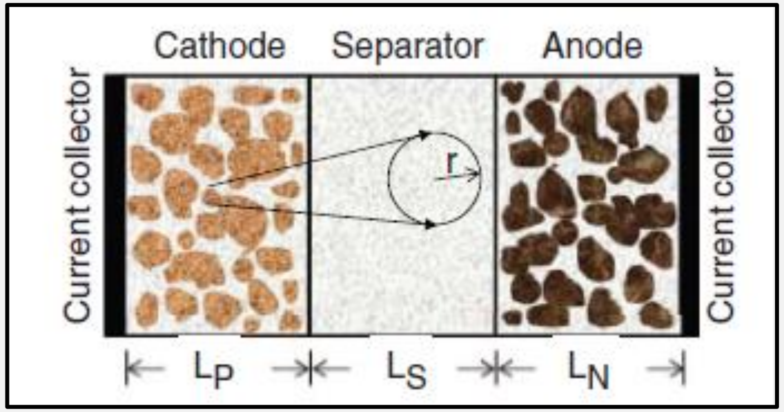
Multiscale Battery Designer



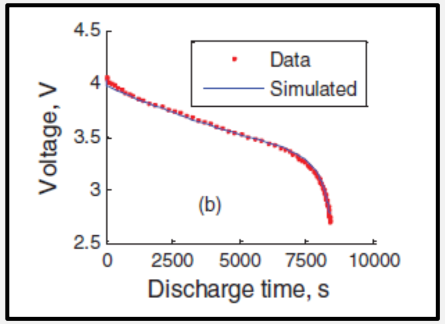
Microstructure



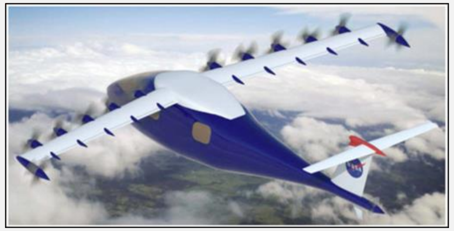
Chemical Design



Cell Design



Cell Simulation



NASA Electric Aircraft

Multiscale modeling from chemistry to materials to cell design and simulation for application specific battery systems

Battery Modeling Briefs

I. Sulfur-selenium cathode electrical conductivity
II. Solid-state electrolytes machine learning screening
III. Battery thermal anomaly prognostics

I. Sulfur-Selenium Cathodes: Electrical Conductivity Computations

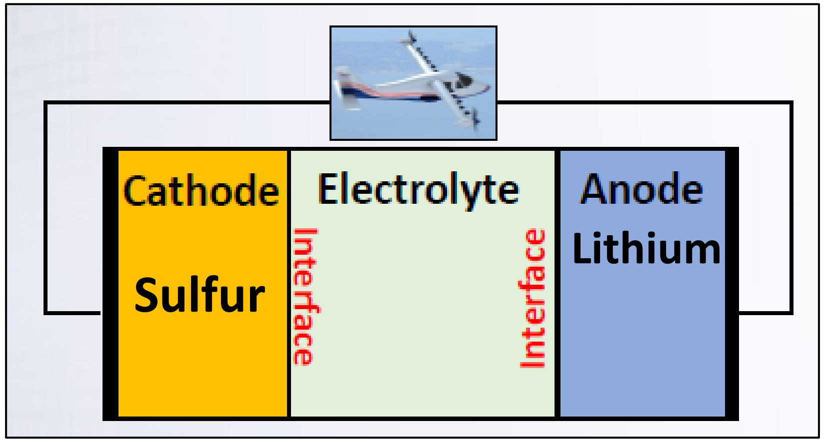
- **Li-S batteries** have high energy density needed for electric aircraft
- **Sulfur cathodes** are poor electrical conductors

  → *Selenium additives* to boost conductivity
- Electron transport in S-Se is poorly understood
  - *Mobility*: how mobile a single electron is
  - *Conductivity* = mobility x carrier density
- **Electron transport mechanisms**:

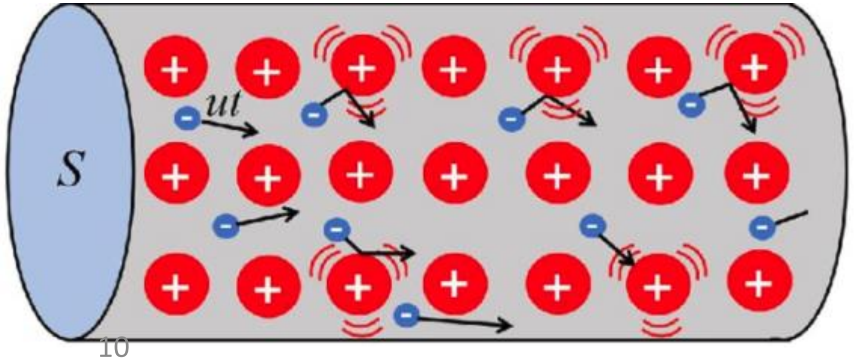
  1) *band transport* (wave)

  2) *hopping* (particle)

High energy density Li-S battery

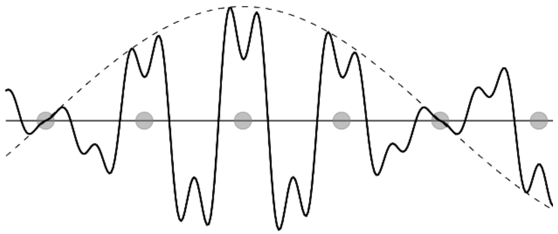


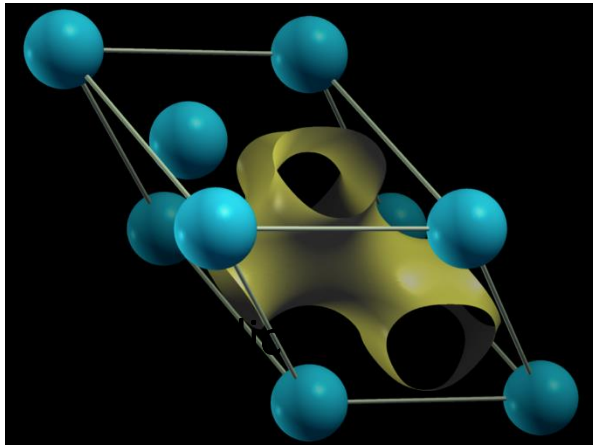
Electron transport in sulfur cathode



S-Se Cathodes: Electron Transport Mechanisms

- **Band (delocalized waves):**



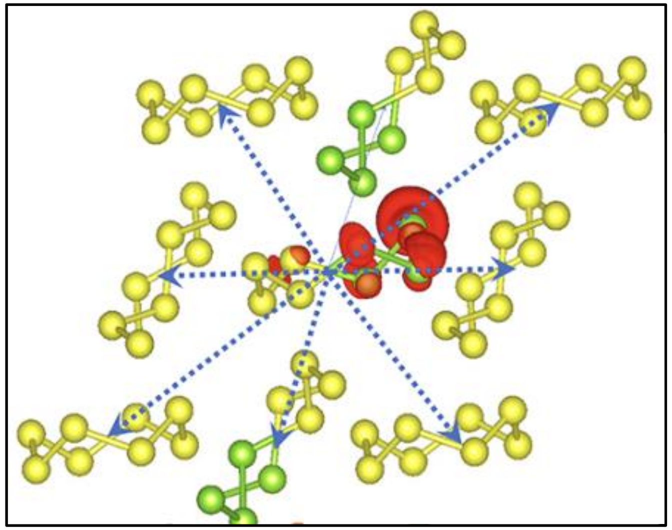


Electron band transport

- Band mobility: $$\mu_{\text{band}} = \frac{q\sum_{\nu\mathbf{k}}(\mathbf{v}_{\nu\mathbf{k}} \otimes \mathbf{v}_{\nu\mathbf{k}})\boxed{\tau_{\nu\mathbf{k}}}\left(-\frac{\partial f}{\partial E}\right)_{E_{\nu\mathbf{k}}-\zeta}}{\sum_{\nu\mathbf{k}} f_{E_{\nu\mathbf{k}}-\zeta}}$$

→ need to calculate scattering rates for each mechanism

- **Hopping (localized particles):**



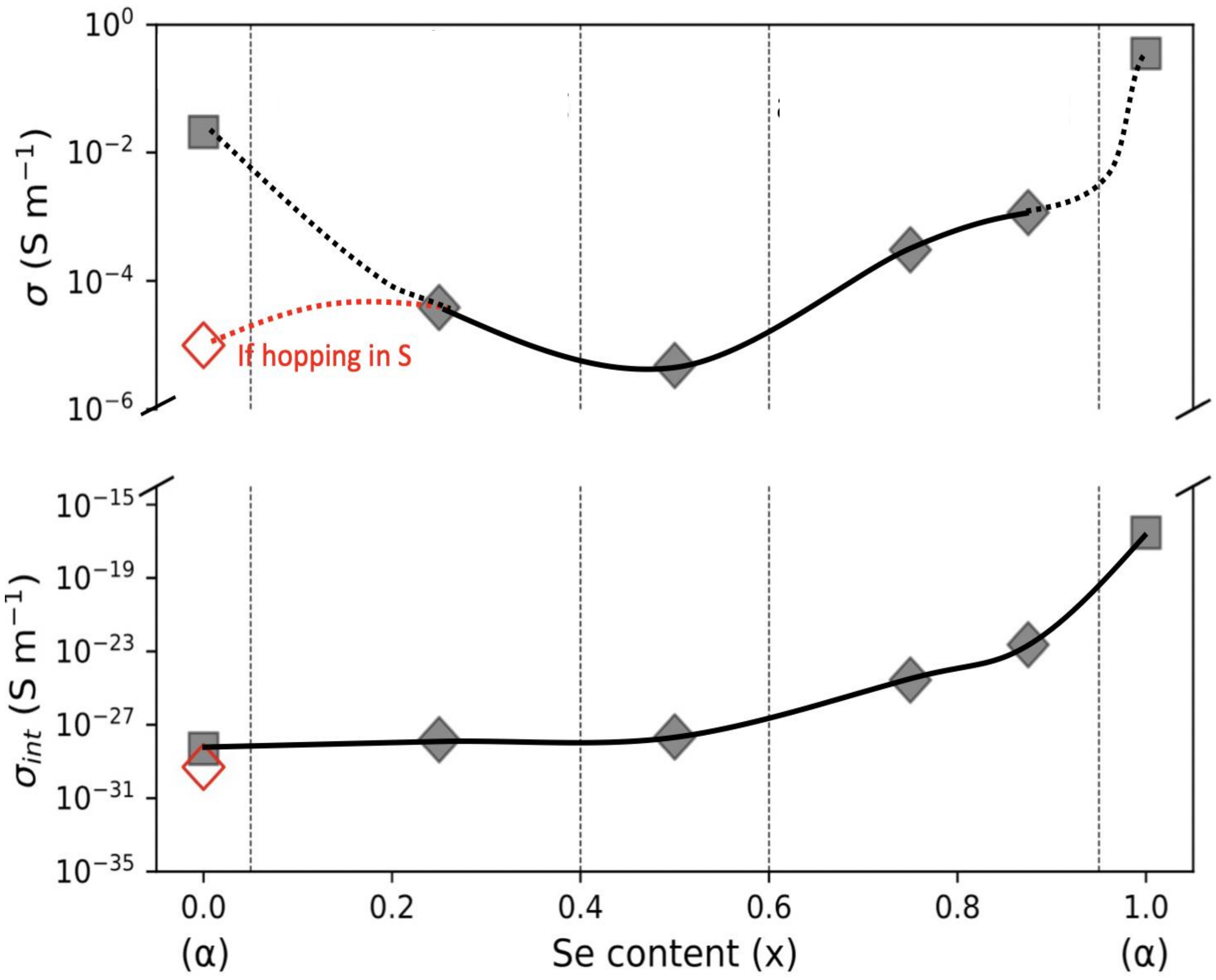
Electron hopping

- Transition Rates:

$$\tau_{ab}^{-1} = \frac{|\mathcal{V}_{ab}|^2}{\hbar^2}\int_{-\infty}^{\infty} \exp\left[i\frac{(E_a - E_b)}{\hbar}t - \sum_{\lambda} S_\lambda\left((2n_\lambda + 1) - n_\lambda e^{-i\omega_\lambda t} - (n_\lambda + 1)e^{i\omega_\lambda t}\right)\right] dt$$

- Mobility is obtained using Monte Carlo

S-Se Cathodes: Electrical Conductivity



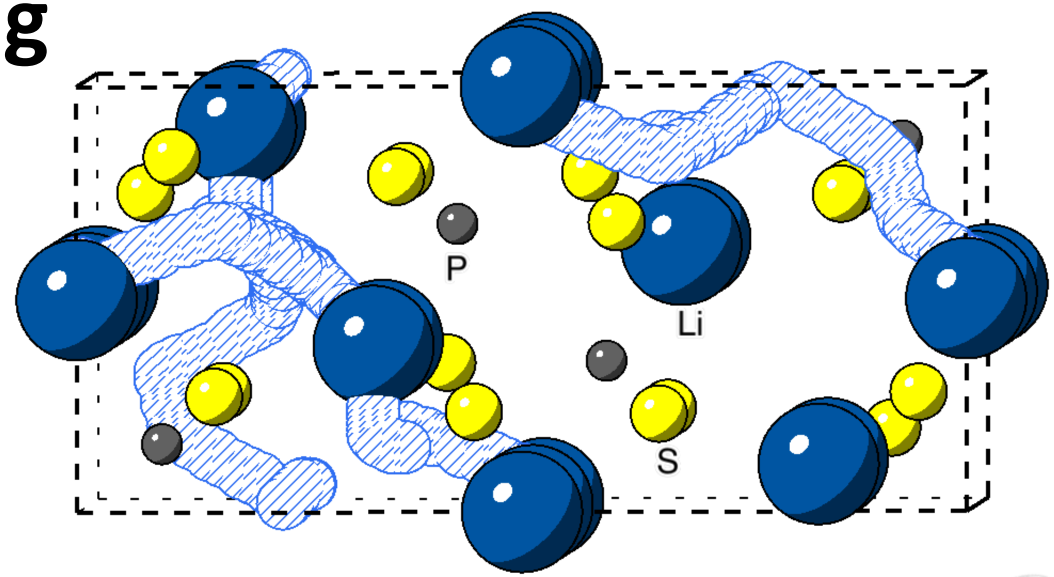
Intrinsic:

- σ increases due to decreasing band gap
- 1~2 order improvement over 50% Se

Doped:

- Pure S could have highest σ, if band transport
- If not, 1 order improvement over 25% Se

II. High-throughput Screening with Machine Learning

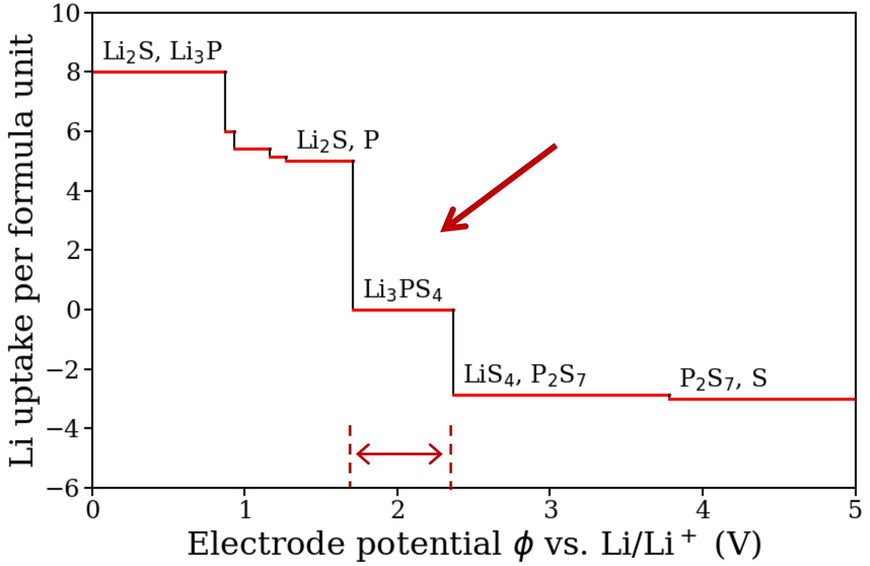


All Solid-State Batteries with Li Anode

- higher safety
- higher energy density
- higher charging rates

Solid-State Electrolyte Requirements

- high ionic conductivity
- low electronic conductivity
- good electrochemical stability
- inertness to air, water
- abundance, low cost, manufacturability etc.



Honrao, S.J., *et al.* Discovery of novel Li SSE and anode coatings using interpretable machine learning and high-throughput multi-property screening. *Sci Rep* **11**, 16484 (2021)

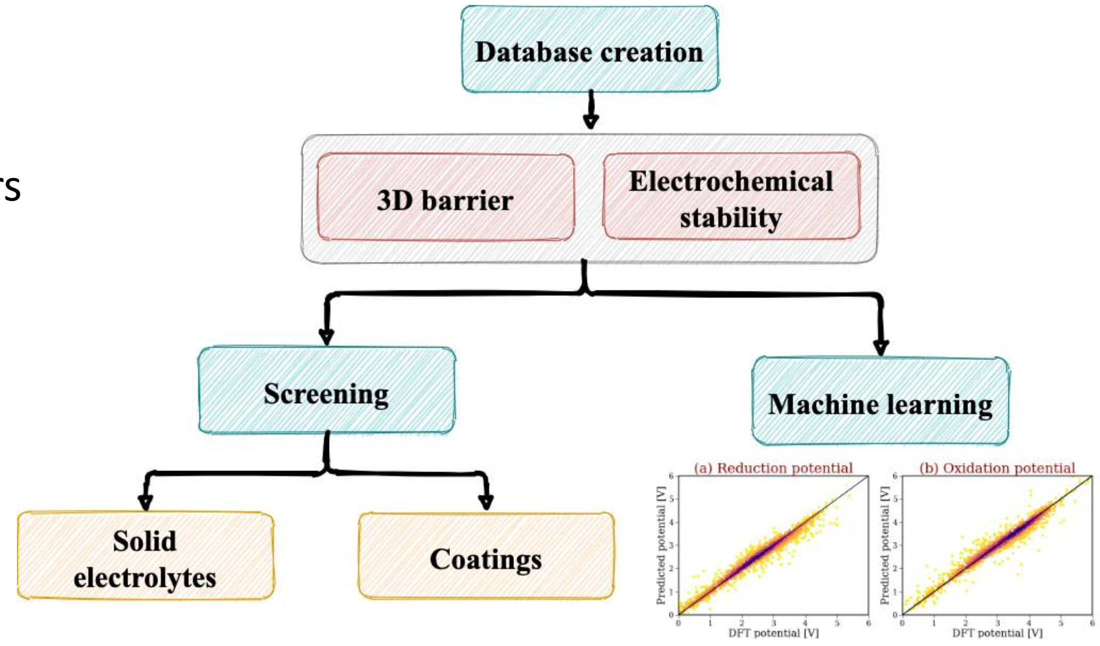
Materials Informatics Approach

- Generate a **database** of battery-related material properties

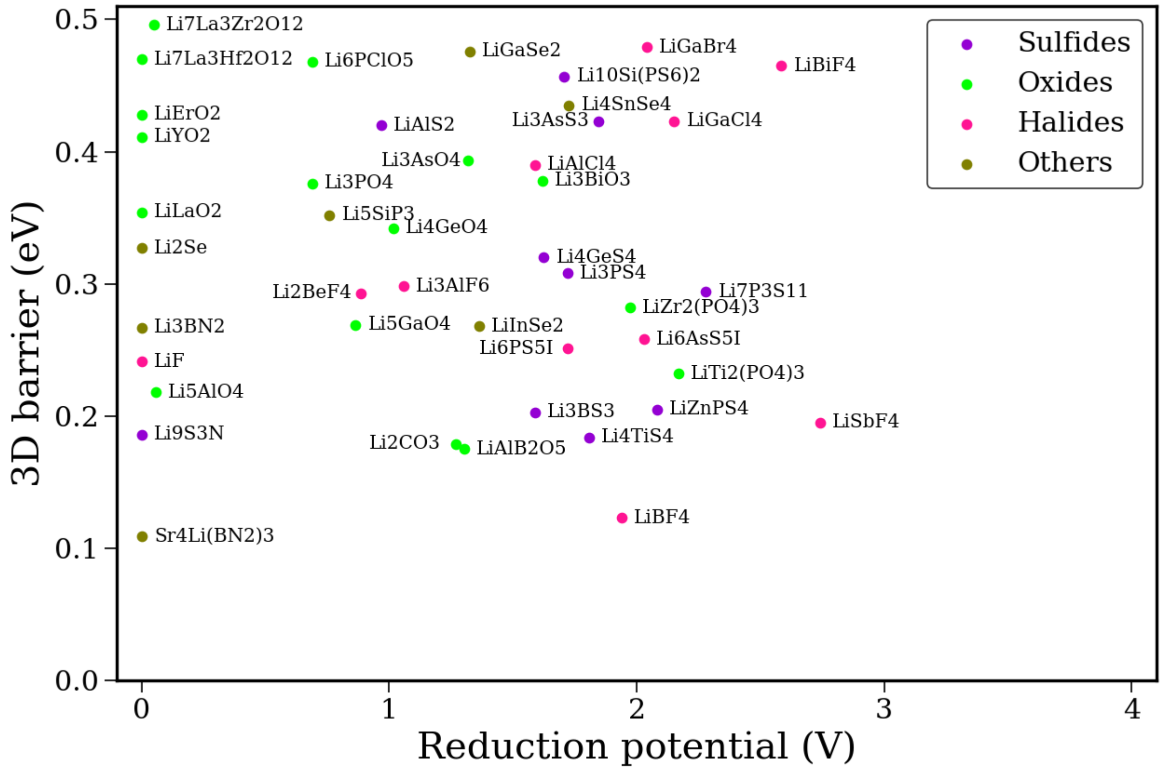
- **High-throughput Screening** through the database for candidates with low Li^+ migration barriers, good thermodynamic and electrochemical stabilities

- Train **Machine Learning** models to predict migration barriers and oxidation and reduction potentials

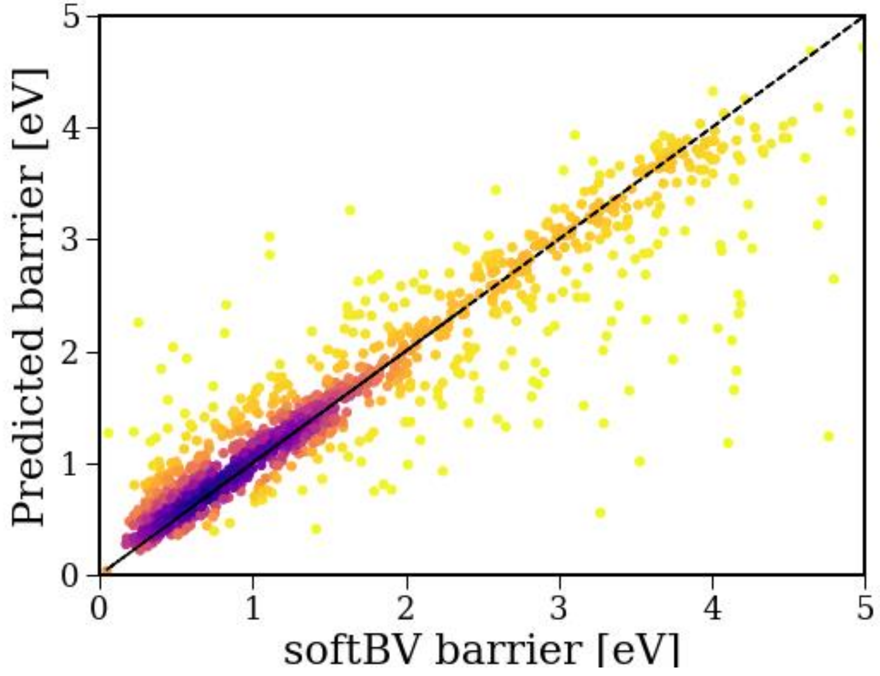
- **Explain** individual predictions and provide **model**-level **interpretation** of feature importance



High-throughput Screening & Machine Learning

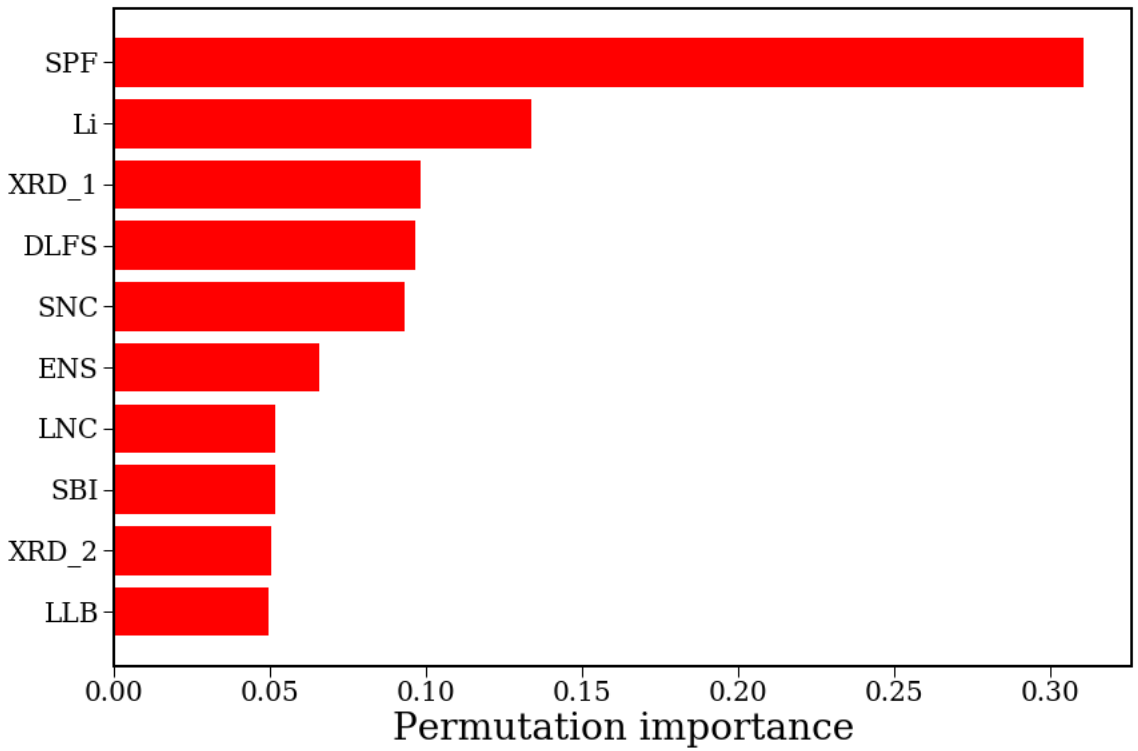


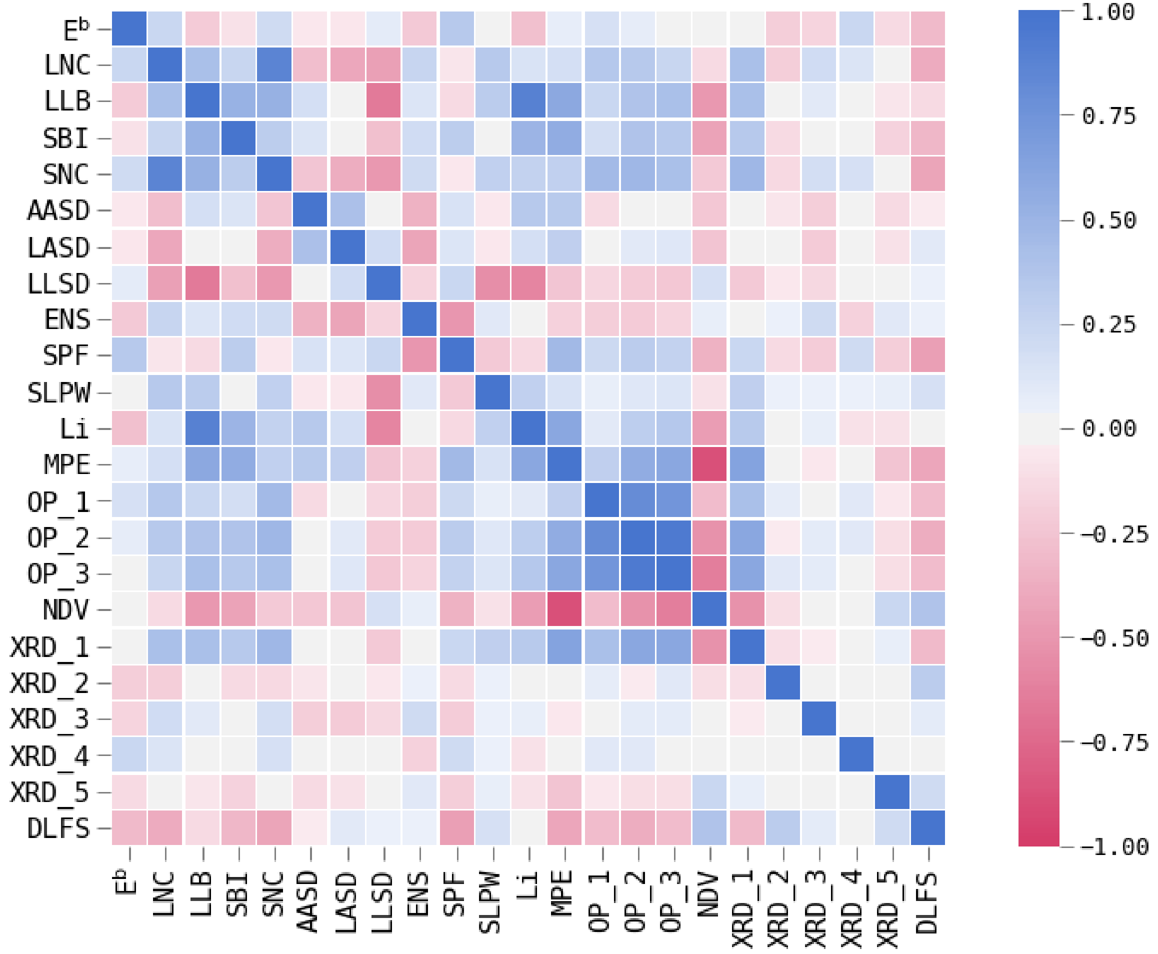
ML model predictions



- **Goal**: identify materials with low migration barriers and good stability
- Machine learning lets us interpolate and extrapolate across available data and make rapid predictions for new candidates

Model Interpretation and Analysis





We can interrogate the machine learning models to better understand why certain materials have better transport or stability than others

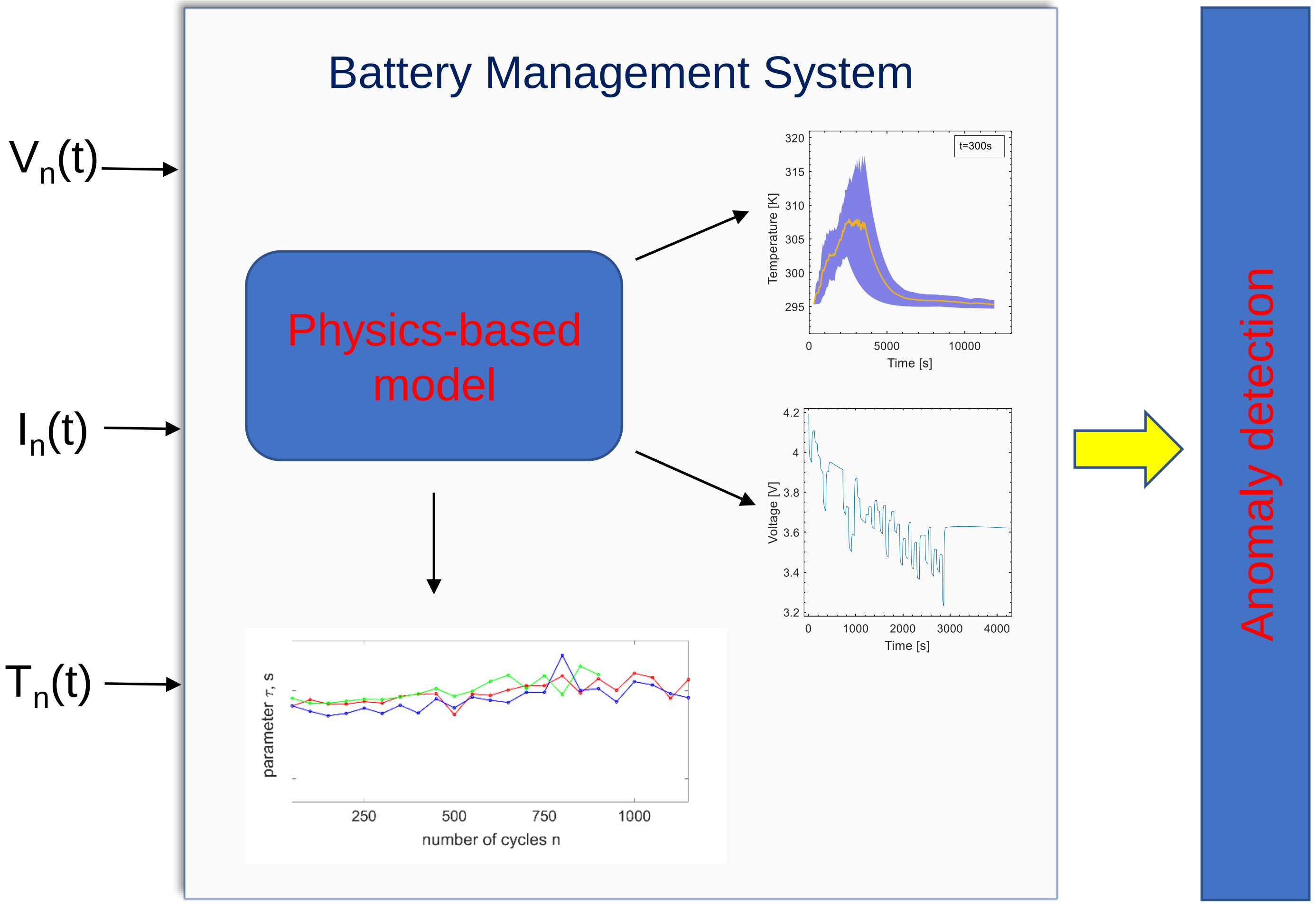
III. Battery Prognostics For Thermal Anomalies

Problem: Thermal runaway is a major safety concern for certification for electric aircraft

Possible solutions:

1. Containment: Bulky packaging - a poor solution for airspace applications: **extra weight!**

2. Prevention: Detecting **early warning signals** for the TR using a BMS.



Outcome: The ability to predict thermal runaway will increase safety and reduce battery weight

Battery State Variables vs Parameters

Hybrid Equivalent Circuit Model

$$V(t) = U_p^0(x_p) - U_n^0(x_n) - \eta'_R - \eta'_p - \eta'_n$$

$$x_i = \frac{(C_{s,i} + C_{b,i})}{C_{max}}$$

$$\dot{C}_{s,p/n} = \pm \frac{\mathrm{i}_{\mathrm{app}}}{F} + \frac{(C_{b,p/n} - C_{s,p/n})}{\tau_D}, \dot{C}_{b,i} = \frac{(C_{s,i} - C_{b,i})}{\tau_D}$$

$$\dot{\eta}'_R = \frac{\mathrm{i}_{\mathrm{app}} R_0 - \eta'_R}{\tau_R}, \qquad \dot{\eta}'_i = \frac{2V_t \sinh^{-1}\left(\frac{J_i}{J_i^0(C_{s,i})}\right) - \eta'_i}{\tau_i}$$

Lumped Thermal Model

$$\frac{dT}{dt} = \frac{I(t)}{C_b}\left(U - T\frac{dU}{dT} - V(t)\right) - \frac{T - T_a}{\tau}$$

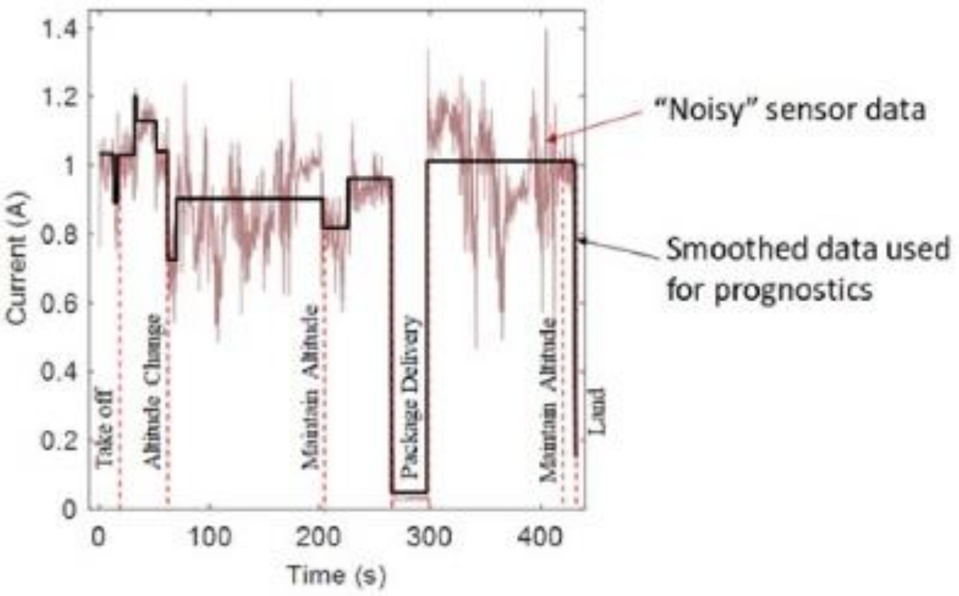
$$\frac{dT}{dt} = \frac{I(t)}{C_b}\left(V_0 - V(t)\right) + \frac{T - T_a}{\tau}$$

- State variables (blue) change during a cycle: fast dynamics (charging/discharging)
- Battery parameters (red) evolve over many cycles: slow dynamics (aging , degradation)

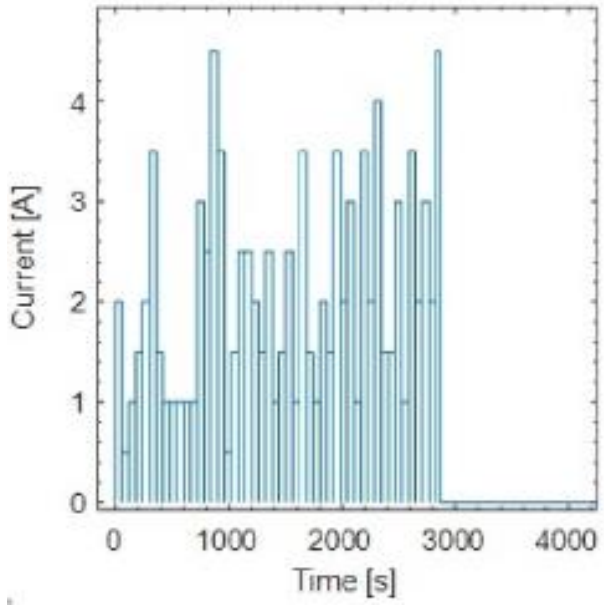
Simulated Flight Profiles (SFP)

- Battery parameter estimation is usually done from lab data.
- **Goal:** battery parameter estimation approach from available field data.
- We use Simulated Flight Profile (SFP) as a proxy to real flight data.

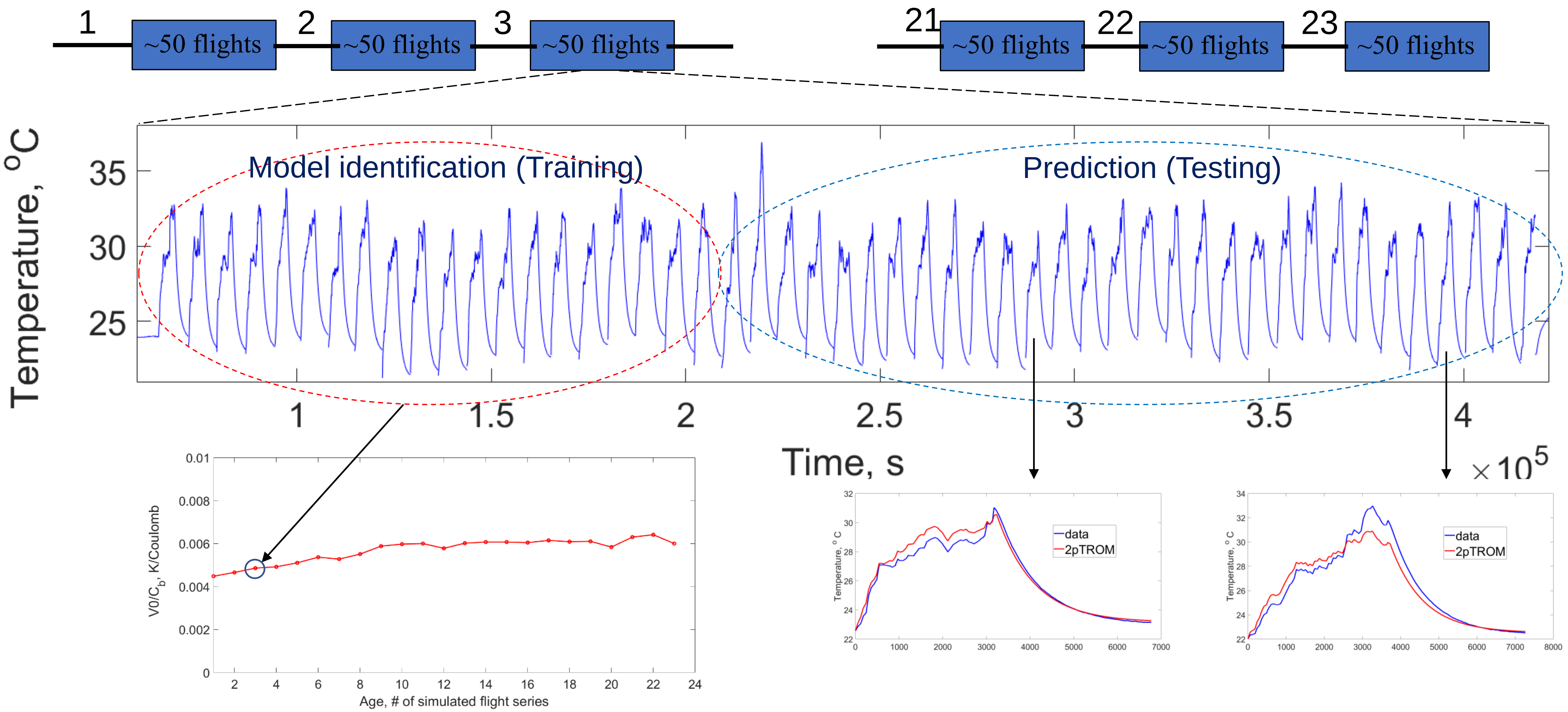
Real Flight Profile



Simulated Flight Profile



Battery Temperature Prognostics with 2pTROM



Summary

- NASA has a vast range of materials issues that can benefit from computation
- Electric aircraft need significant advances in batteries
- We have a multiscale, multi-pronged set of activities including
- First principles
- Data science
- Multiphysics modeling
- Prognostics