LiON: Li-O_2 Batteries for NASA Electric Aircraft

NASA: *John Lawson* (ARC), Vadim Lvovich (GRC), Kurt Papathakis (AFRC)

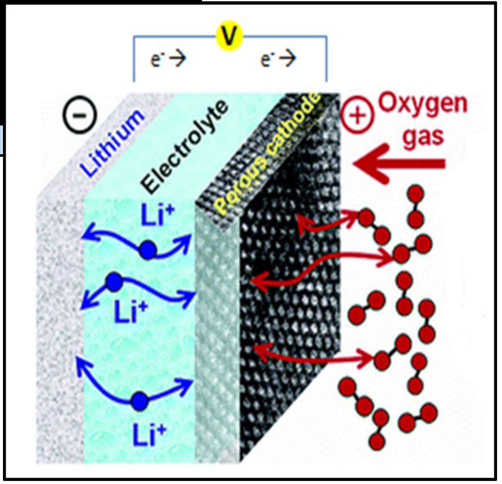
External Partners: UC Berkeley, Stanford, Carnegie-Mellon, IBM Almaden, ARL, ORNL, Purdue, Colorado School of Mines, UC San Diego

NASA Strategic Plan for Green Aviation

Strategic Thrust 4:
Transition to Alternative Propulsion and Energy

- Zero emissions
- Low noise
- Energy efficient

Li-Air Battery

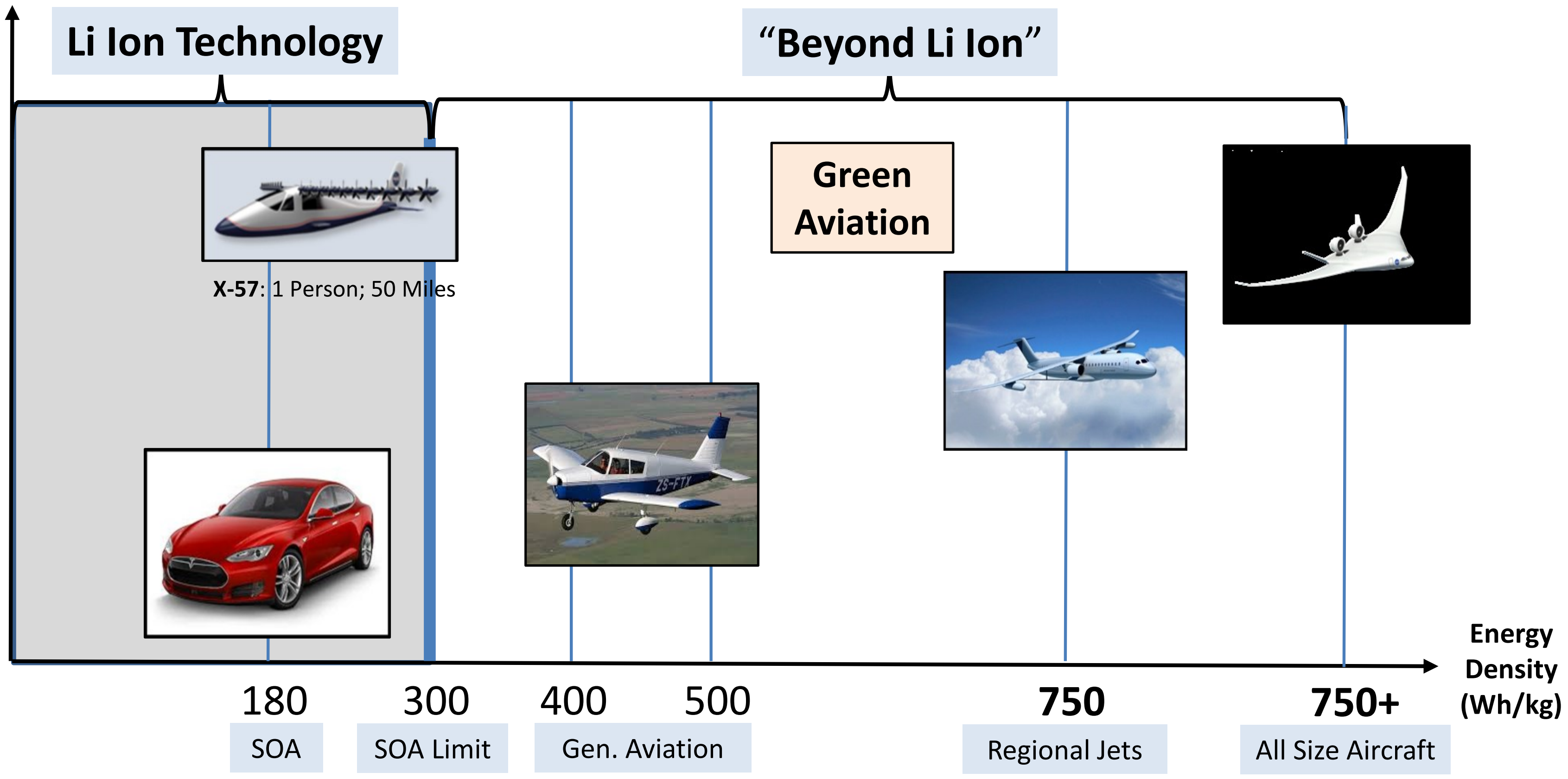


Batteries are a critical enabler for electric aircraft

Green Aviation Battery Requirements

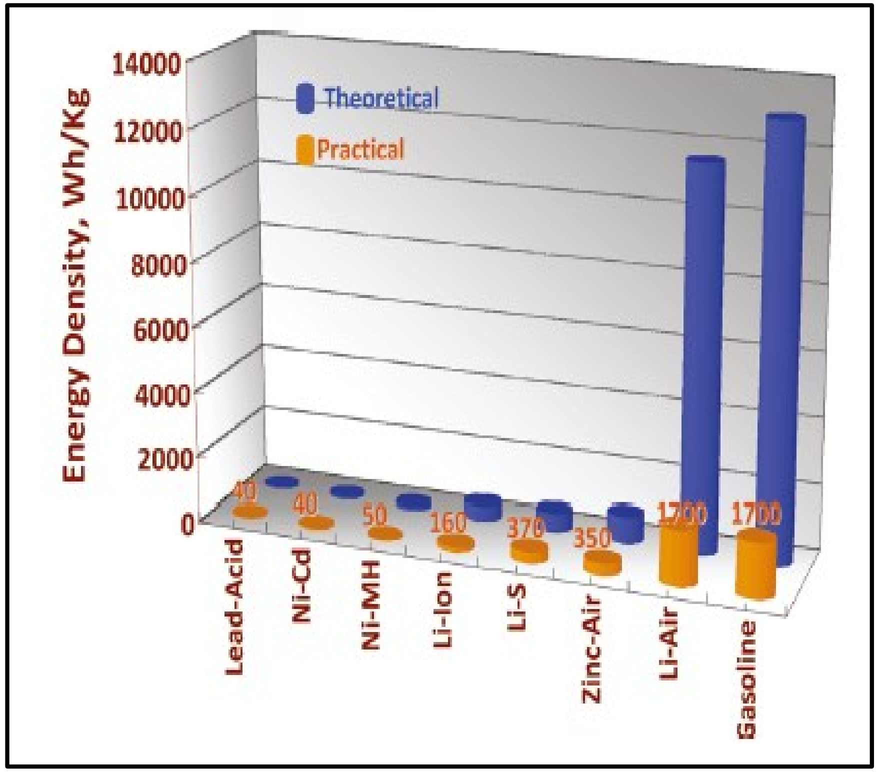
Major requirement is: High Energy Density

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

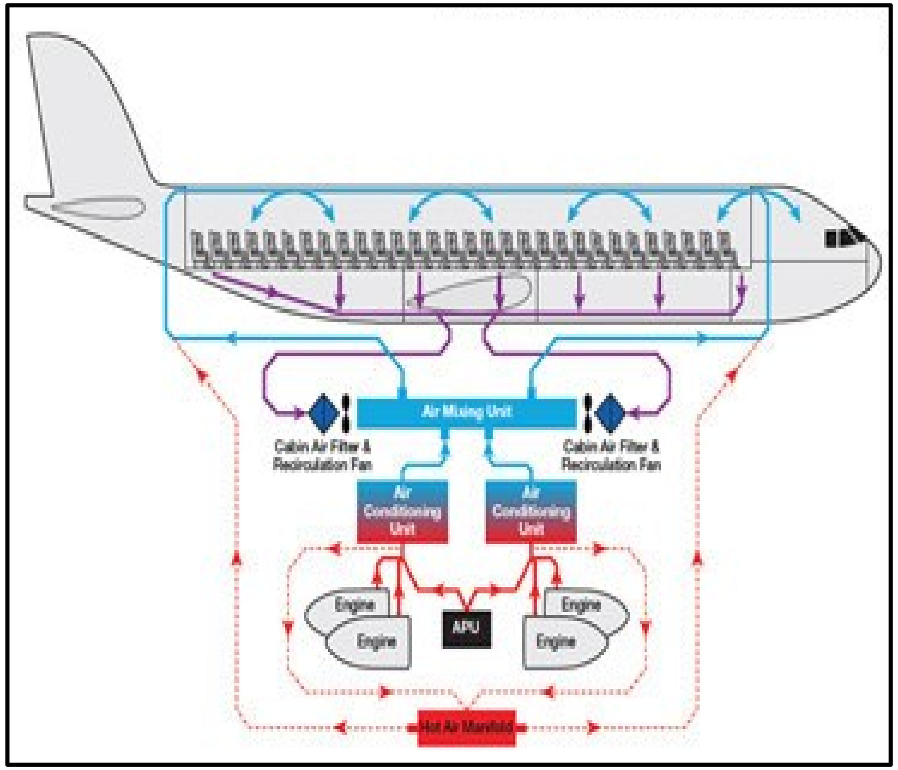


Electric aircraft have the most extreme requirements of any battery application

Li-Air is Unique Fit for Electric Aircraft

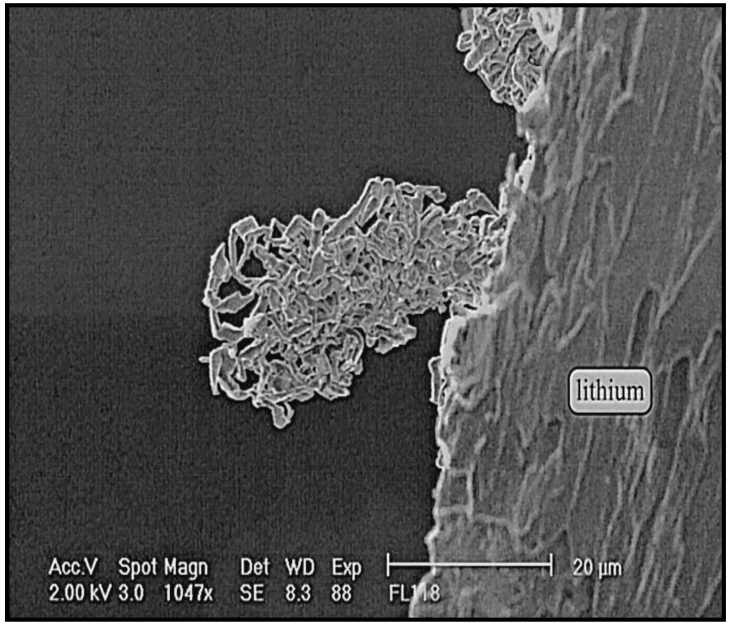


Li-Air has <u>highest</u> theoretical energy density.
Very few alternatives.



Aircraft on-board oxygen systems can be leveraged for Li-Air batteries further mass reduction

Major Li-Air Challenges



Electrolyte **decomposition** limits energy density and rechargeability

SOA electrolytes are **flammable**
Unacceptable for aircraft

Electrolytes are the limiting factor for Li-Air batteries to achieve:
- Practical high energy densities
- Rechargeability
- Safety

LiON Technical Thrust Areas

		State of the Art	Transformative
I	**Computation**	Empirical "*trial-and-error*" method	Predictive computation to accelerate development
II	**New Materials**	Commercial "*off-the-shelf*" materials	New material components designed and fabricated
III	**Mechanisms**	Decomposition mechanisms poorly understood	Mechanism informed "*Electrolyte Design Rules*"
IV	**Electric Flight**	Academic, laboratory studies	Electric aircraft flight systems integration

Multidisciplinary approach integrating computation, synthesis/fabrication and application engineering needed to make rapid progress for complex technologies such as batteries

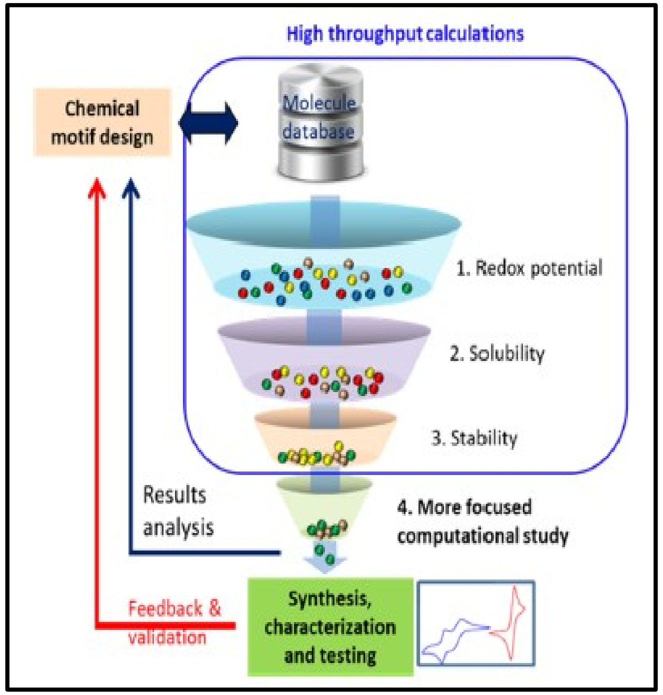
Accomplishments

- Multiscale Battery Modeling
- Material Evaluation: Electrolytes
- Material Design I: Electrolyte Stabilizers
- Material Design II: High Stability Electrolytes
- Material Design III: High Stability Cathodes
- Li-Air Pack for Electric Aviation

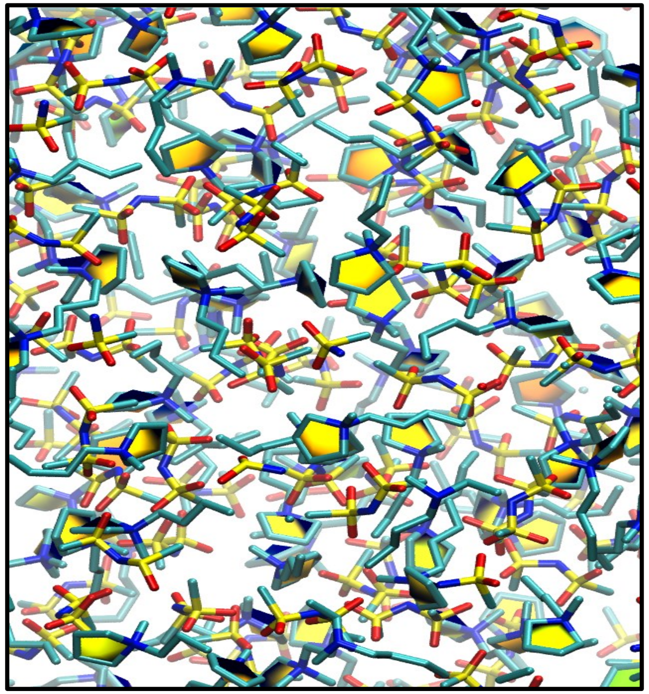
Multiscale Battery Modeling

SOA Li-Air research uses highly empirical “trial-and-error” approach

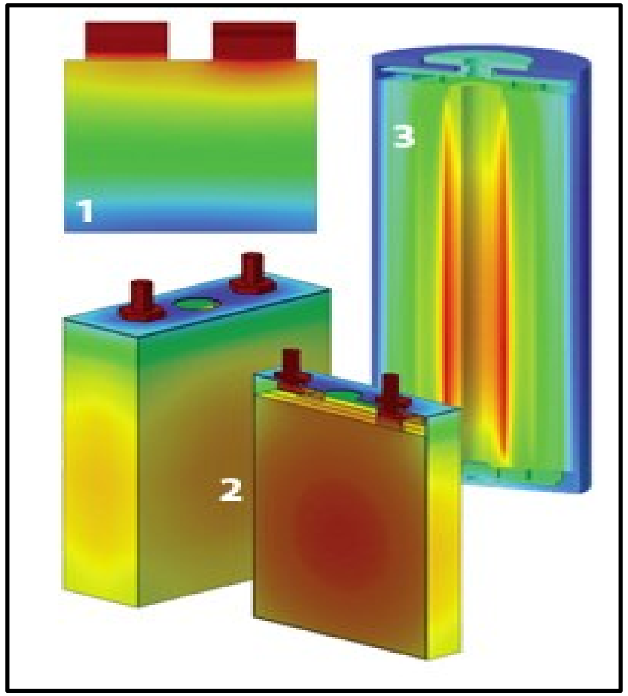
Vision 2040



High-throughput screening



Materials simulations



Multiphysics analysis

We used predictive modeling at multiple scales leveraging NASA supercomputing to accelerate development

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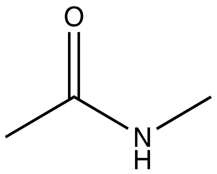
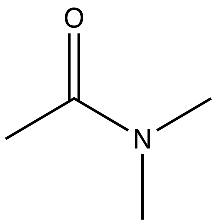
Material Evaluation: 10 Organic Electrolytes

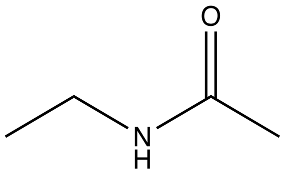
Amides



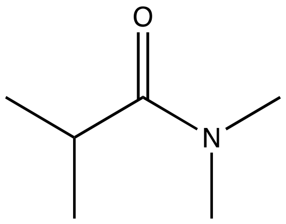
NMA



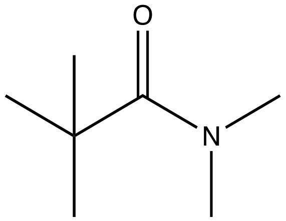
DMA



EMA

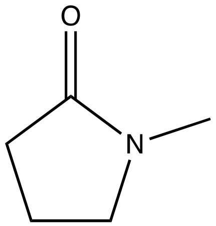


DMDMA

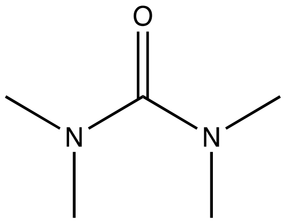


TMDMA

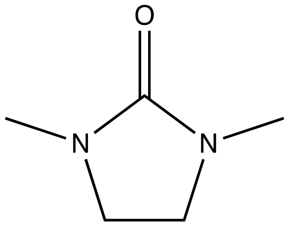
Ureas



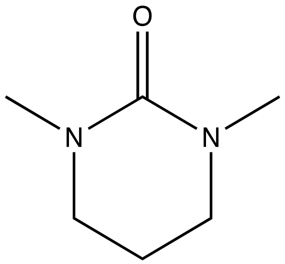
NMP



TMU

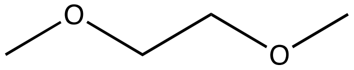


DMI



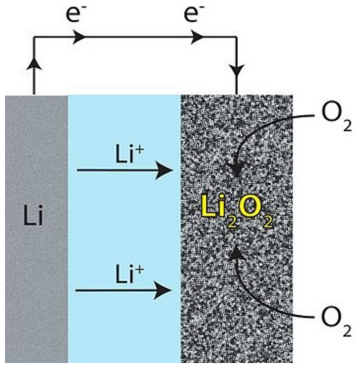
DMPU

Ethers

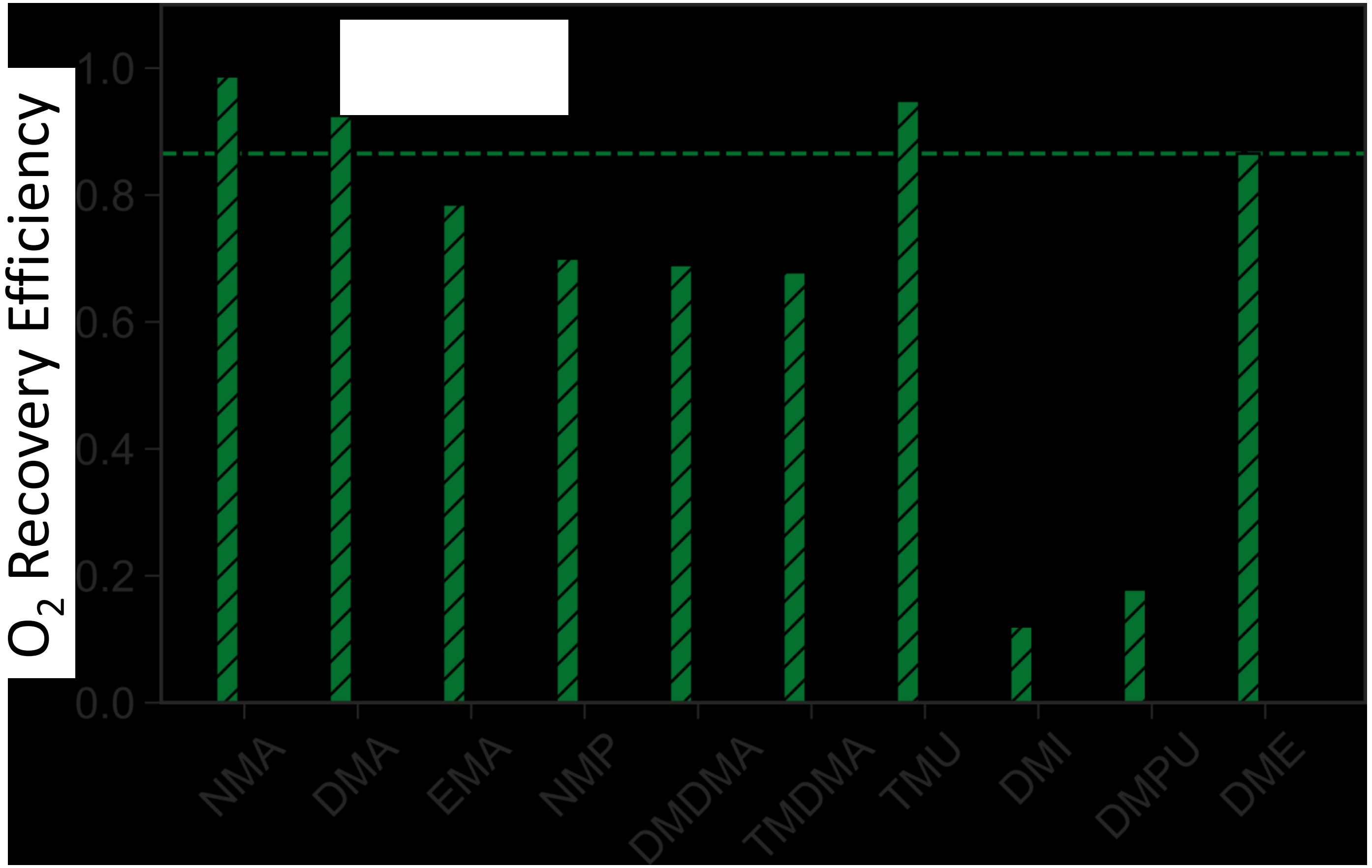


DME

Amides and Ureas expected to perform better than SOA Ethers

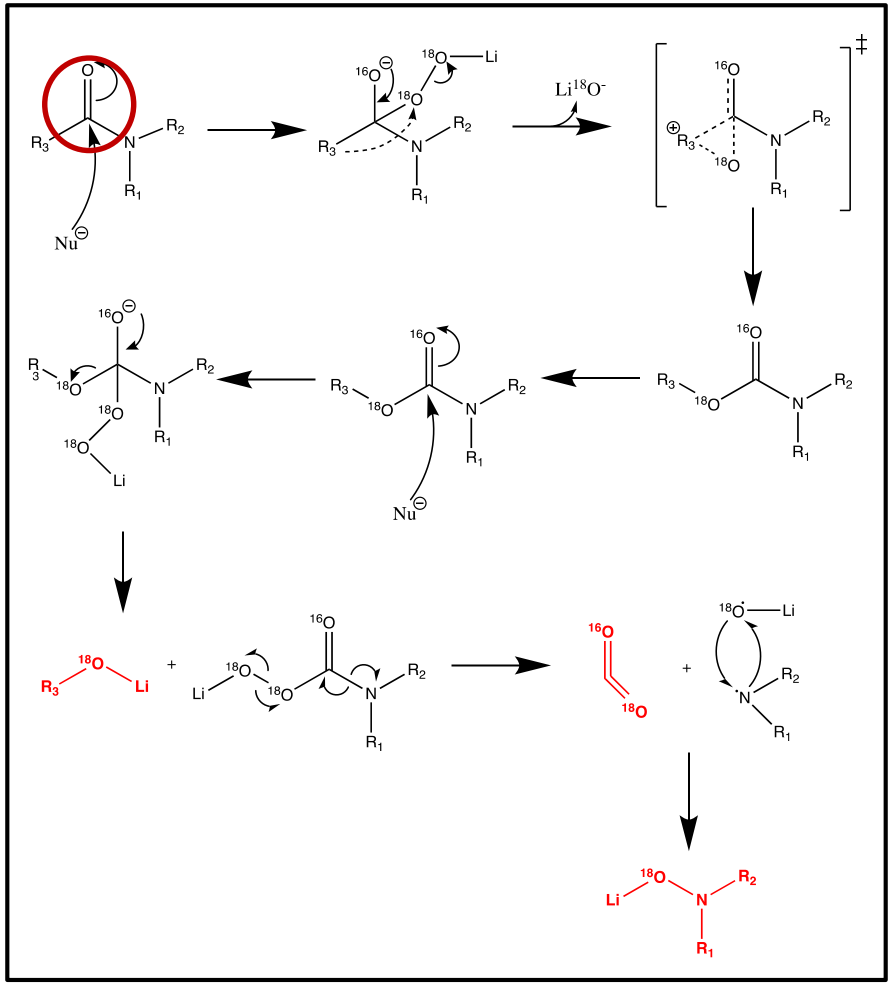


Oxygen Recovery Efficiency



Efficiency determines cycle life: 100 cycles requires 99.9% efficiency

Decomposition Mechanisms Discovered



Mechanism identification suggests stability design rules: protect C=O bond

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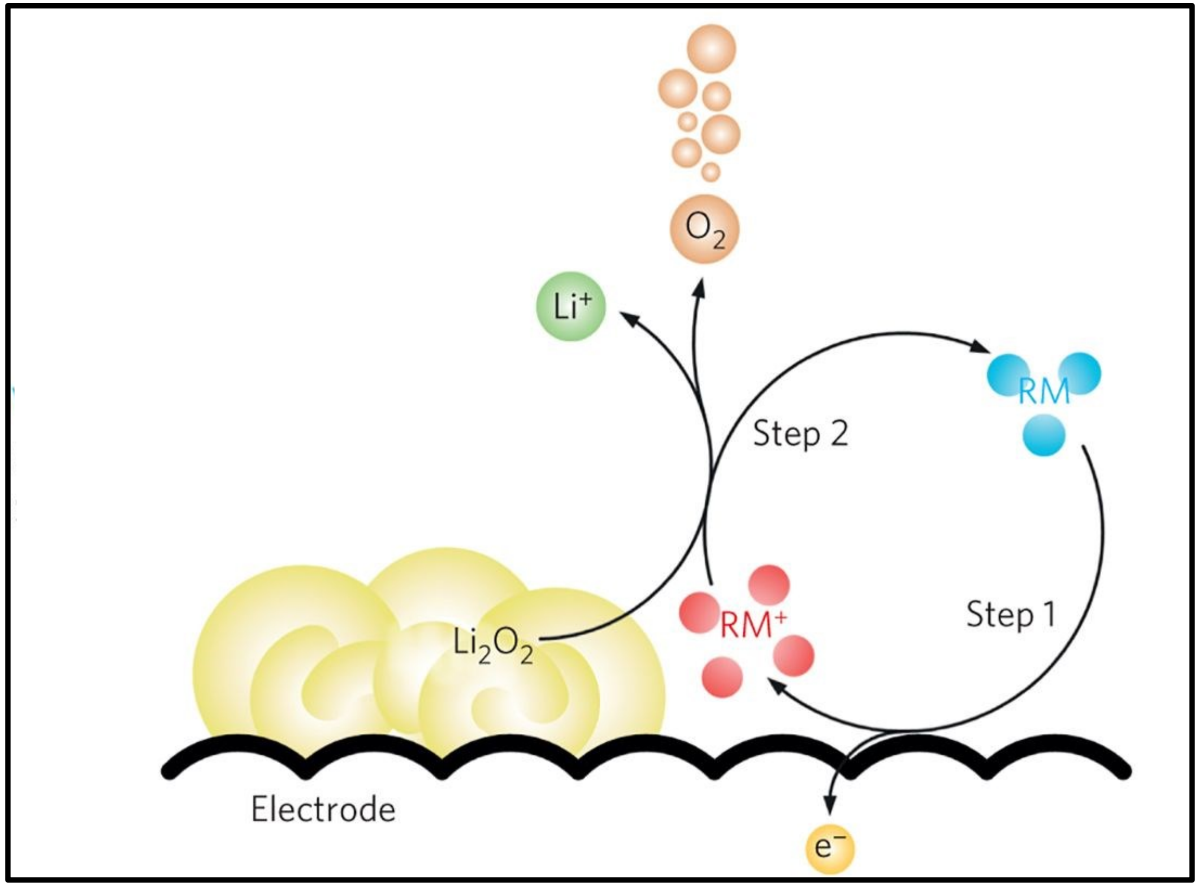
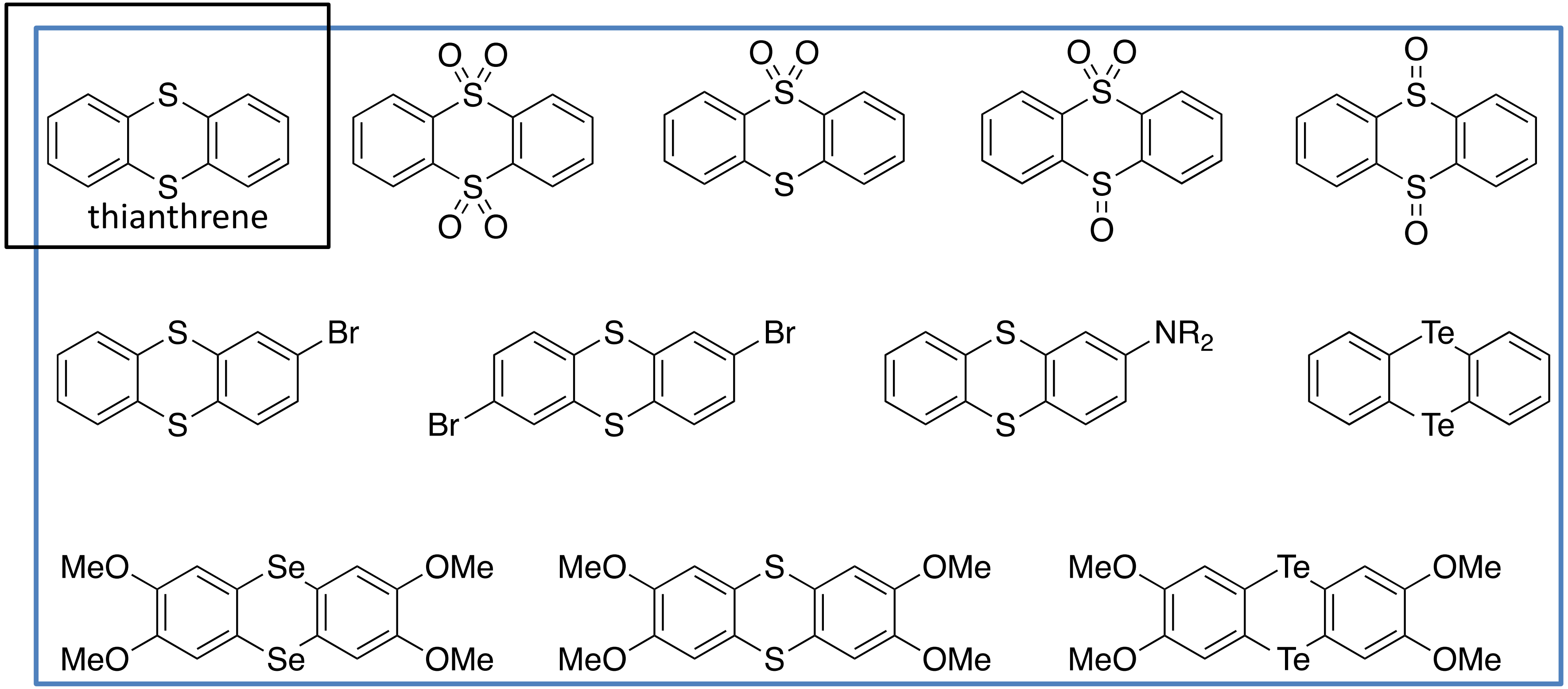
Electrolyte Stabilizers



Stabilizers release locked up O_2 increasing O_2 recovery efficiency

Tunable Electrolyte Stabilizers



- Properties ***tuned*** by varying substituents, e.g. $=O_2$, -Br, $-NR_2$, etc.
- Computational screening to down select best candidates
- ***2X*** improvement in cycle life

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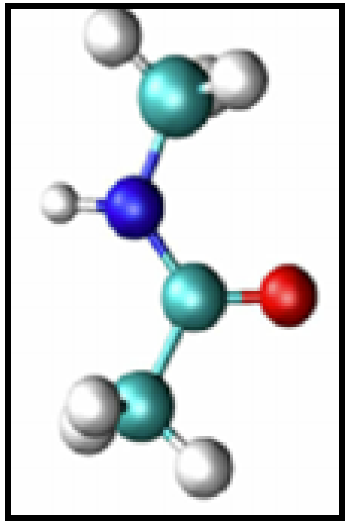
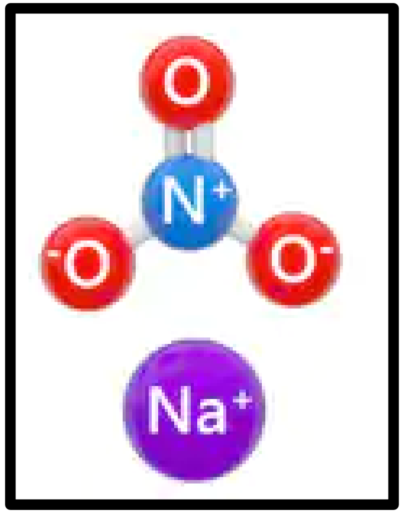
Going Inorganic: Molten Salt Electrolytes

Organic Electrolytes

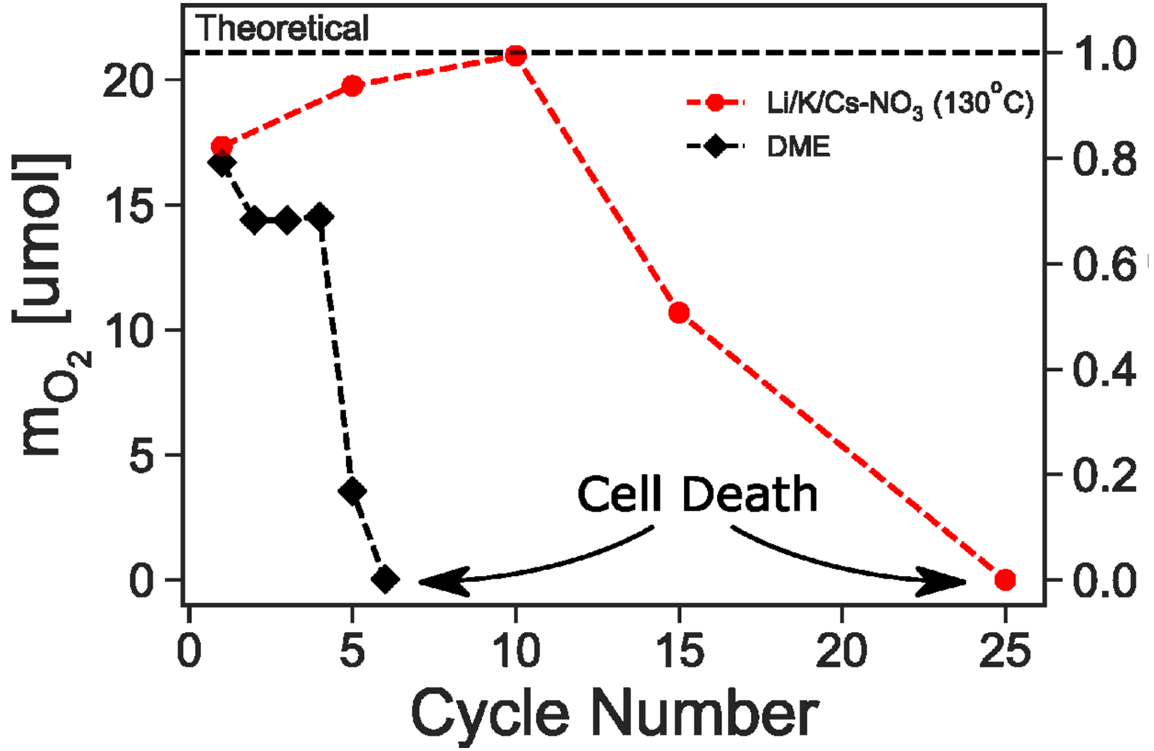


Molten Salt Electrolytes



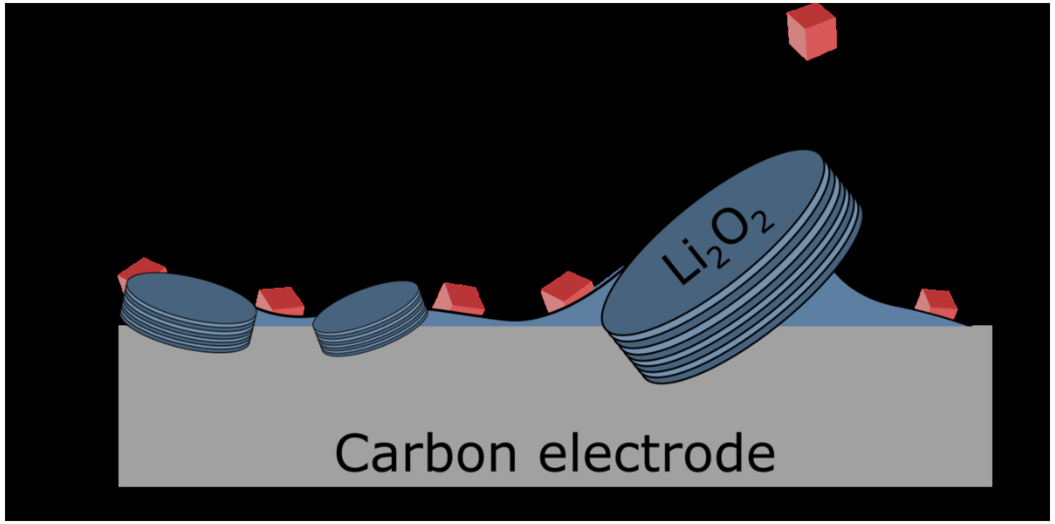
- Persistent decomposition issues with organic electrolytes
- Inorganic molten salt electrolytes tried for improved stability

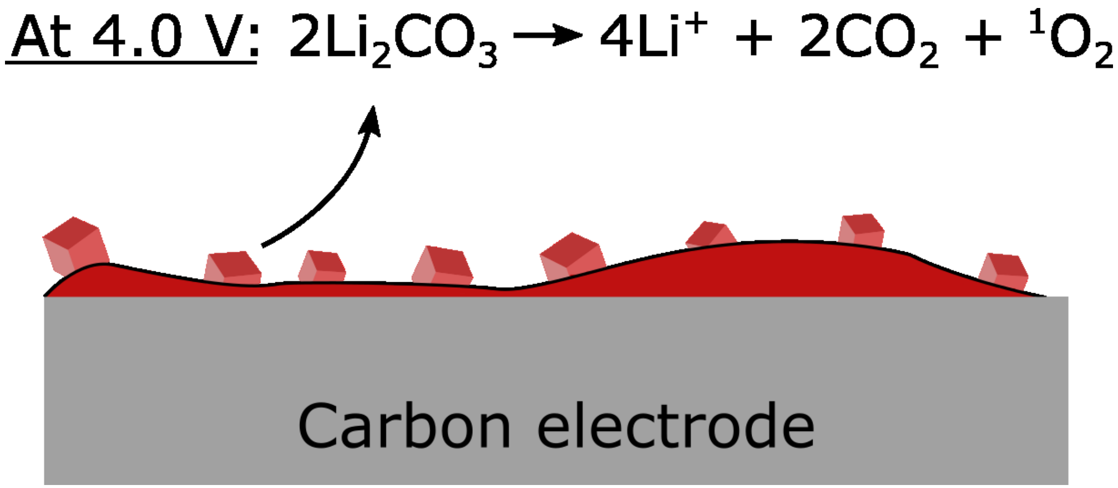
Molten Salt Electrolytes: Cycle Life



<u>*5X*</u> increase in cycle life with molten salt electrolytes vs SOA (DME)

Cell Death with Carbon Cathodes





Parasitic product Li_2CO_3 forms *insulating* layer on electrode killing the battery

Thus, high stability electrolyte and high stability cathode required

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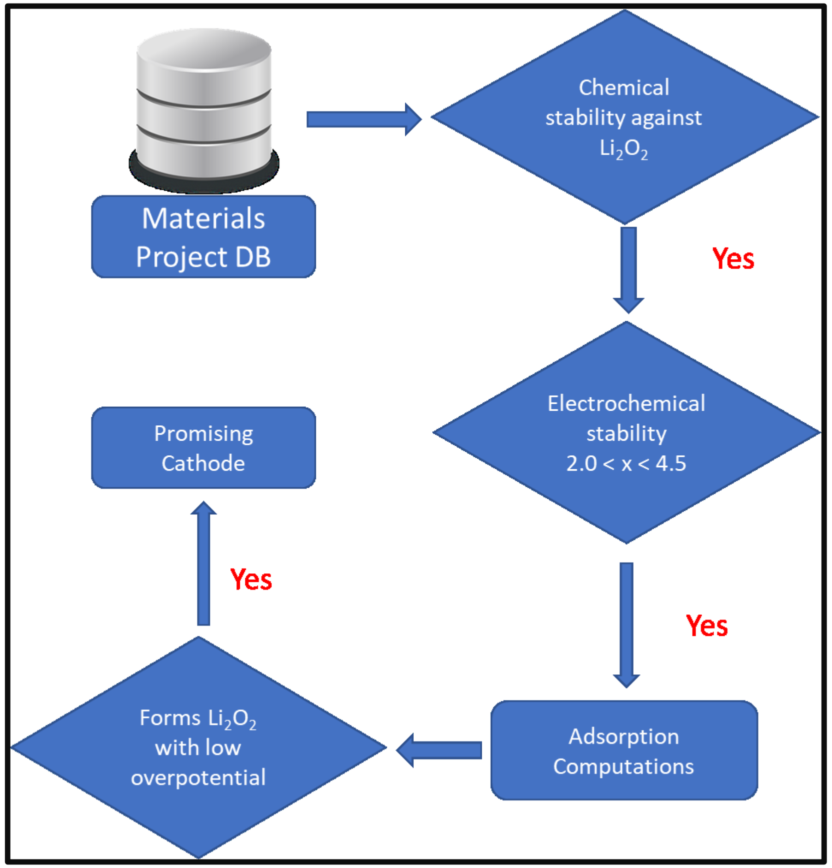
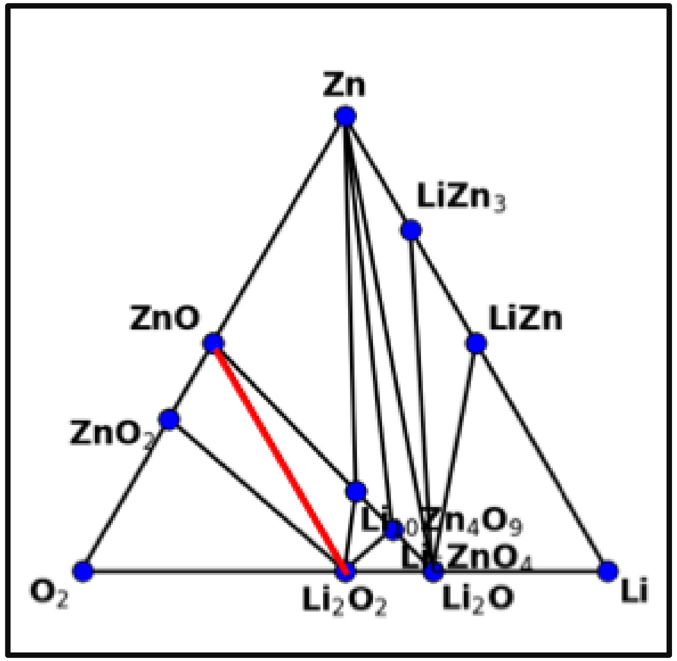
Computational Screening: Cathode Materials

High Throughput Workflow

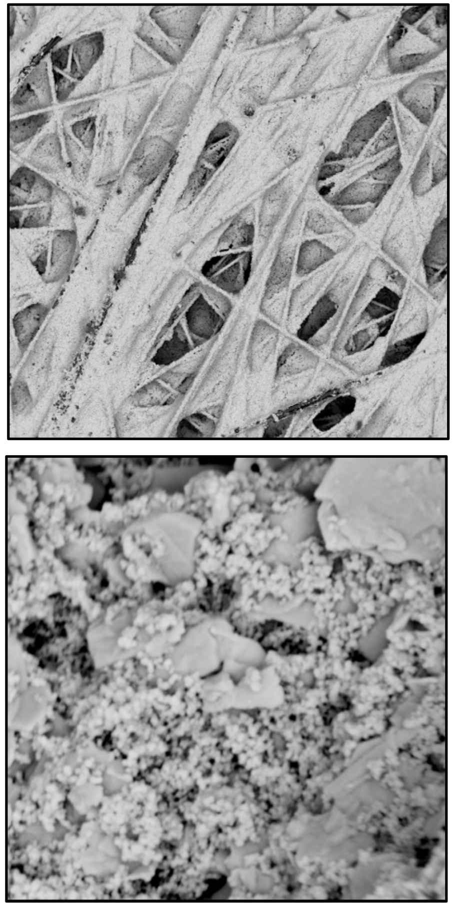


Phase Diagrams

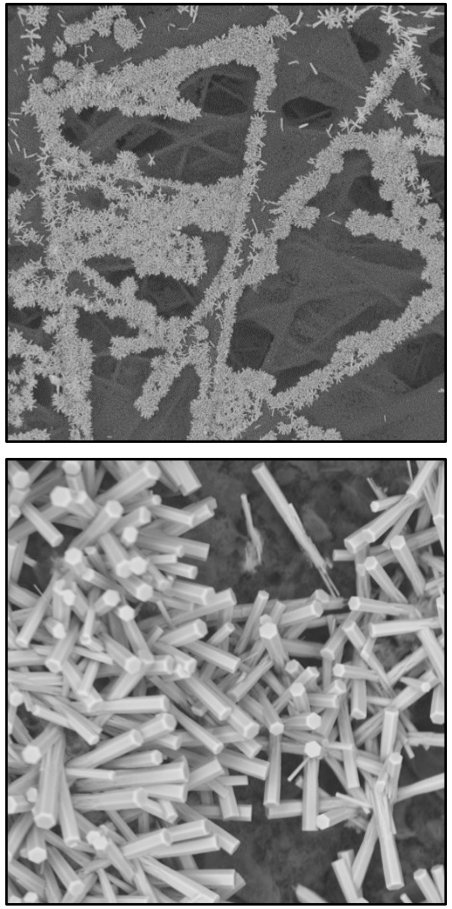


Can we find cathode materials more stable than carbon?

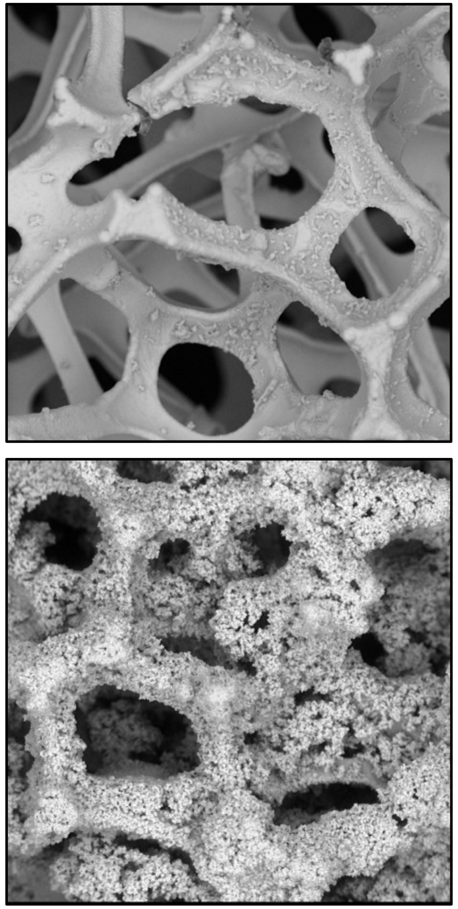
Cathode Design



RF Sputtering-P50



Hydrothermal-P50



Hydrothermal-Ni Foam

- Many cathode materials (ZnO, ATO, ITO, etc) fabricated and tested
- Dramatic, *unexpected* parasitic processes observed – batteries fail after *one* cycle
- Materials are promising but require further work

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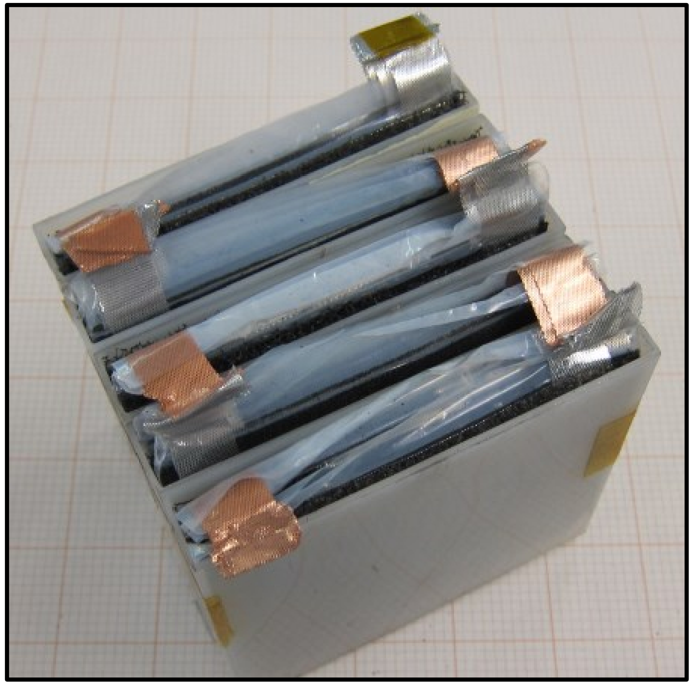
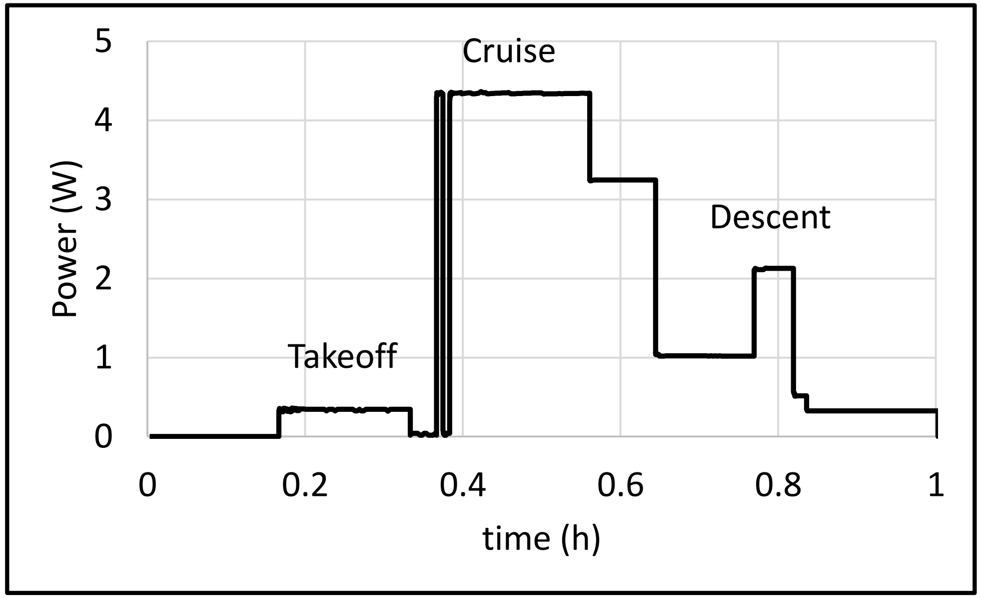
Li-Air Battery Pack



5-cell, 12-Volt pack (300 grams)



$Li\text{-}O_2$ battery pack performed well for electric flight power profile test

Further work to increase specific power (W/kg) and volumetric power (W/L)

Conclusions

- **Material design approach identified a promising path to extended cycle life** and higher practical energy densities for Li-O_2, involving alternative electrolytes, stabilizers, new cathodes, etc.
- **Li-O_2 is viable for electric aircraft**. Given enormous potential and very limited options (Li-O_2, Li-S, etc.), Li-O_2 should be on the table for future development.
- **Li-O_2 is still fundamentally a low TRL technology** and significant development required for it to be deployed in real applications.
- **NASA can and should contribute to battery development for aircraft**. Not being addressed by DOE or industry who are focused on battery cost and safety for automobiles
- **Multidisciplinary team** combining predictive computation, material synthesis/fabrication, battery engineering and application systems engineering (aircraft) essential to make progress