Sandia National Laboratories

DEVELOPMENT OF A STABLE, HIGHLY WATER-SOLUBLE BI-REDOX MOLECULE FOR AQUEOUS FLOW BATTERIES

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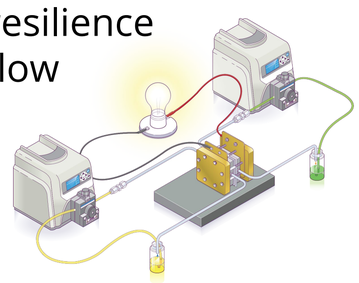
PROJECT PROFILE
Topic: Flow Batteries | Vertical: Materials and Systems Innovation
Strategic Pathway: Optimize & Grow
Project start and finish: FY25-FY27

PROBLEM

- Flow batteries offer a pathway to grid resilience
- Vanadium is the standard in aqueous flow batteries
  - V is expensive with few domestic sources
- Development of **earth-abundant** active materials with **high energy density** and molecular stability is critical to lower consumer cost.



$$\text{Energy Density (ED)}_{RFB} = \tfrac{1}{2} n F V_{cell} C_{active}$$

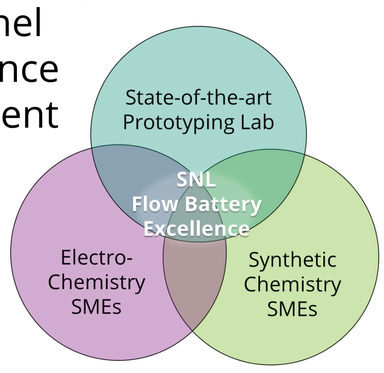
(moles e^-, Faraday Const., Cell Voltage, Active Material Concentration)

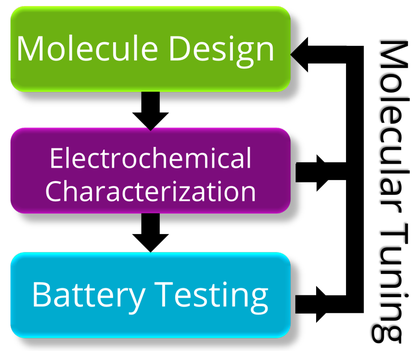
$$ED_{Theoretical,\ SNL\ BRM} = \tfrac{1}{2}(1)(26.8)(1.04)(2) = 27.8\ Wh/L$$

$ED_{Vanadium} \approx$ 20-35 Wh/L

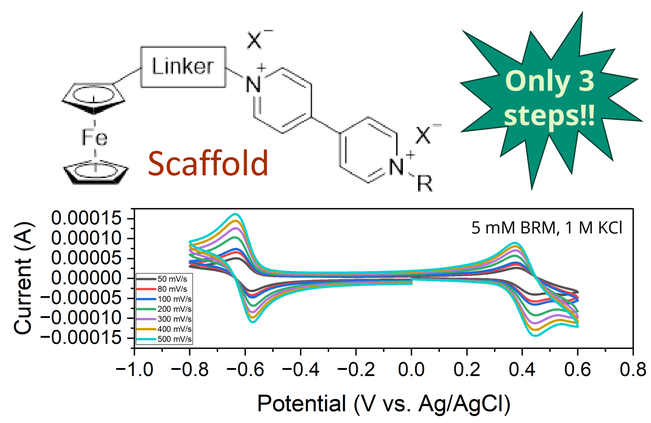
APPROACH

- SNL is uniquely positioned to perform this work due to:
  - Personnel
  - Experience
  - Equipment





Synthesis/E-Chem



BRM Testing

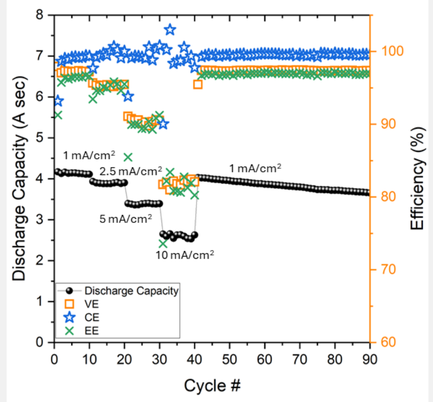


Fig. 1. General molecule scaffold & cyclic voltammograms (left) and battery cycling curves (right)

RESULTS

The key to high solubility & exceptional cell voltage lies in the way the redox species are linked together

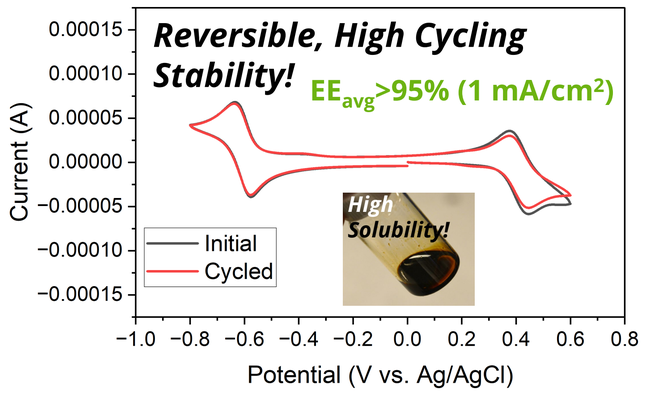
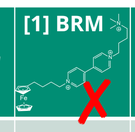


Fig. 2. Cyclic voltammograms of BRM before and after cycling, inset shows highly concentrated (>2M) BRM solution

Table 1. Comparison of SNL BRM to literature-reported BRM

Parameter	[1] BRM 	SNL BRM
Water Solubility (M)	1.2	>2 ✓
Cell Voltage (V)	0.7	1.04 ✓
Capacity fade (%/cycle) @10 mA/cm²	0.00625	0.00024 ✓

CONCLUSIONS & IMPACT

Our BRM possesses the exceptional quality of the gold standard all-Vanadium FB design (symmetric + highly stable) with the added benefits of:

- Neutral pH electrolyte
- Earth-abundant active material
- Less temperature sensitivity

A lower cost energy storage device will have tremendous impact on multiple industries.

Technical advance filed: TAQ1308

FUTURE DIRECTIONS

Future work will include:

- Optimization of BRMs in aqueous flow batteries
- Establishing protocols for widening the voltage window closer to that of all-Vanadium

References

[1] Zhu, Y., et al. (2019). Enhanced cyclability of organic redox flow batteries enabled by an artificial bipolar molecule in neutral aqueous electrolyte. *Journal of power sources*, *417*, 83-89.

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