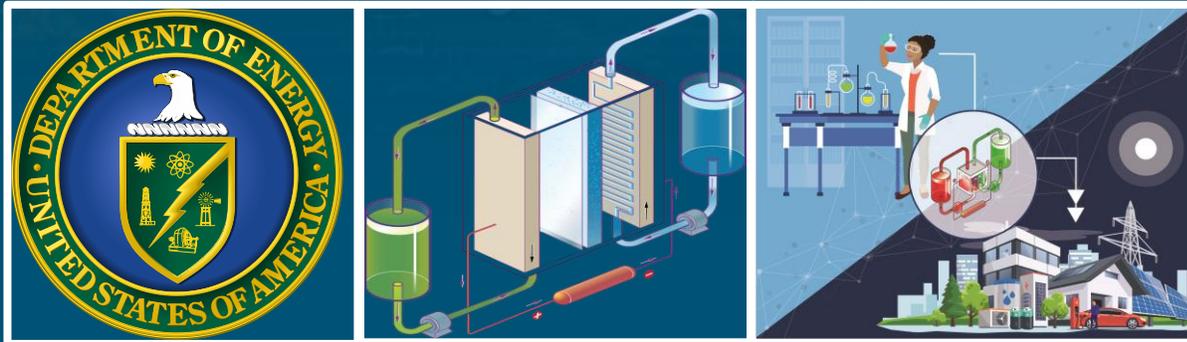


Metal Coordination Complexes for Symmetric, Non-aqueous Flow Batteries



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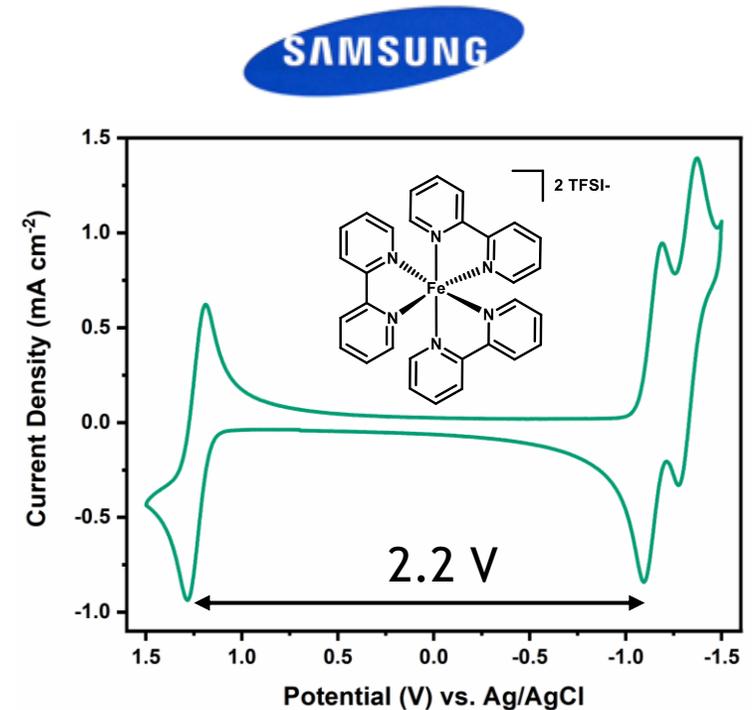
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2 Project Approach and Goals

The Samsung non-aqueous flow battery shown here uses an **earth abundant** iron-bipyridine metal coordination complex (MCC) as both positive (iron) and negative (bipyridine) to **mitigate crossover issues**, but a **higher-voltage** is needed to effectively compete cost-wise with the aqueous vanadium and organic chemistries.

We attempted to chemically modify the bipyridine with electron-donating groups (EDG) and electron-withdrawing groups (EWG) **to achieve a goal of a 2.6 V cell**. We tested the new compounds in both symmetrical and asymmetrical cells to understand battery performance. We discovered **significant negative degradation**.

Our second **goal is to elucidate and mitigate** the negative degradation. The following slide summarizes our results which were published in ***Dalton Transactions* and featured on the back cover**.



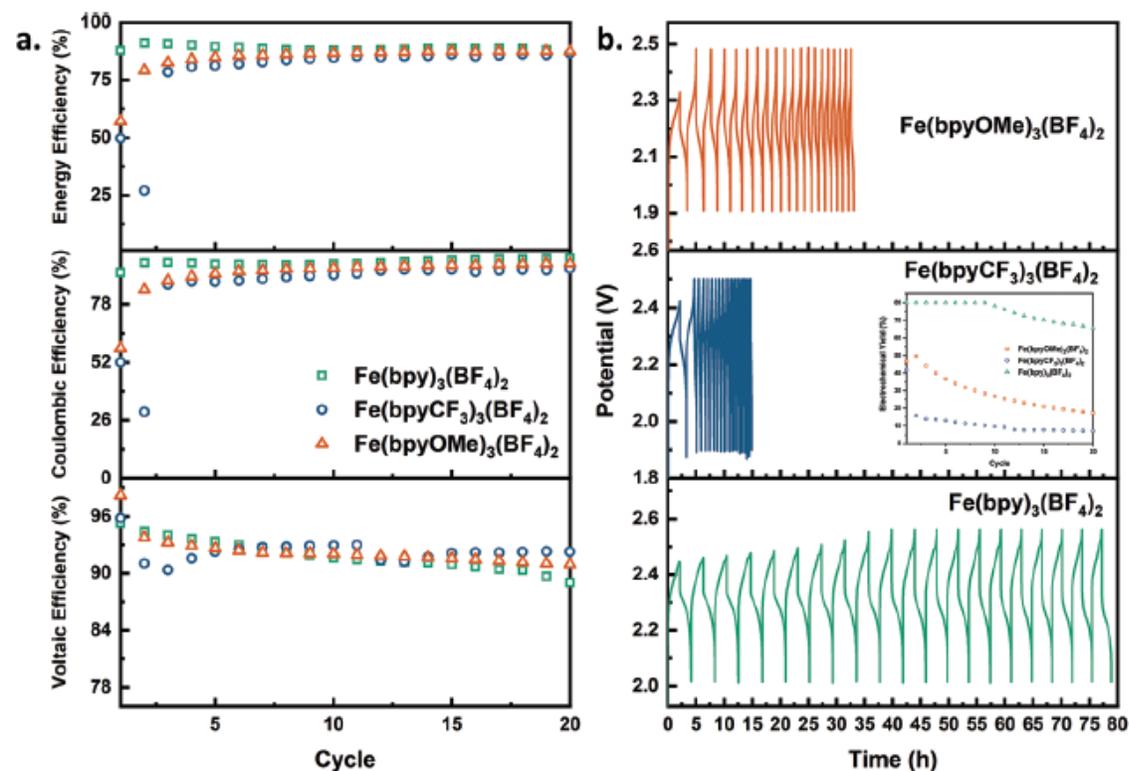
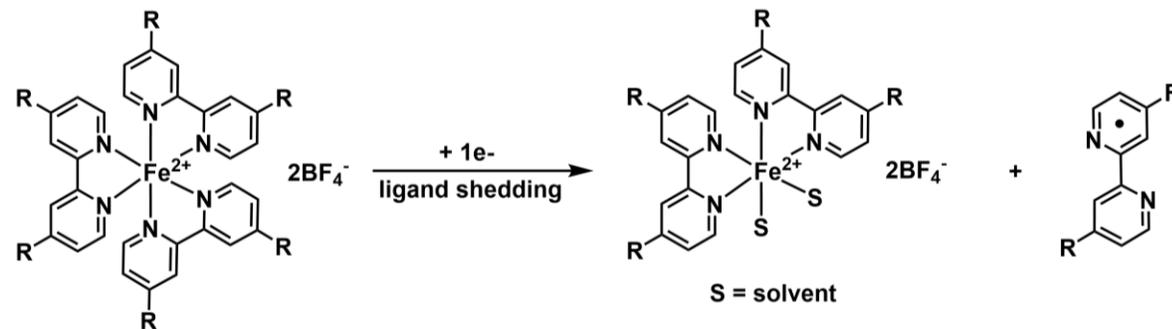
3 Chemically Modified Iron-bipyridines for Symmetrical Flow Batteries



We optimized conditions for rapid screening of MCCs and identified that tetra-ethyl-ammonium/tetra-fluoroborate in propylene carbonate works optimally for commercially available anion exchange membranes (**Dalton Accomplishment #1**).

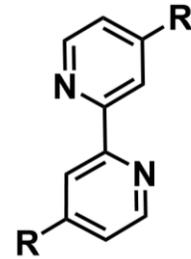
We analyzed the effect bipyridine substituents have on cycling. The parent compound showed the least capacity fade, indicating that while the modifications could increase voltage, they also increased capacity fade (**Dalton Accomplishment #2**).

We elucidated the cause of capacity fade by testing both symmetrical and asymmetrical cells. All of the cells showed anode degradation which is caused by ligand shedding, exacerbated by the EDG and EWG substitutions, and subsequent irreversible oxidation of unsubstituted ligands (**Dalton Accomplishment #3**).

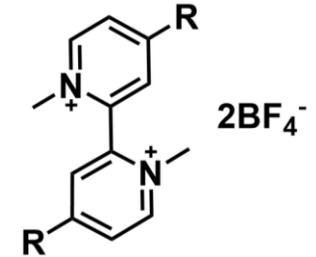


We have launched a new study of **earth abundant non-aqueous organic molecules** as a way to avoid ligand shedding and negalyte degradation. When paired with the iron-bipyridine polysilyte, they create **pseudo-symmetric cells** which also mitigate crossover issues. FY22 will continue to explore these systems.

metal-free molecules



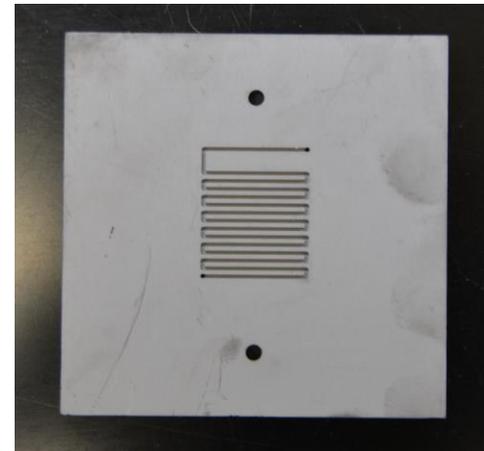
R = CF₃, OMe



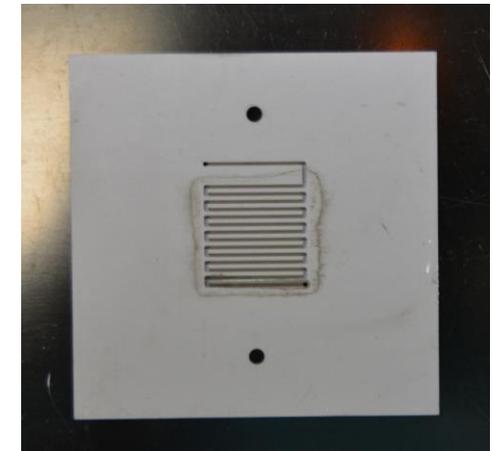
R = H, Me, OMe, CO₂Me

Graphite exfoliation is a known degradation pathway with carbonate solvents. Non-aqueous flow batteries have the advantage over the acidic VRB of being able to **utilize stainless steel** in place of graphite. Rapid prototyping of various flow fields with additive manufacturing has allowed us to accelerate the adoption of stainless steel into non-aqueous RFBs.

Pre-cycled



Post-cycled



Shunt currents cause edge corrosion in the non-aqueous RFBs



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