Optimization of a High Performance Nonaqueous Organic Redox Flow Battery Via Machine Learning

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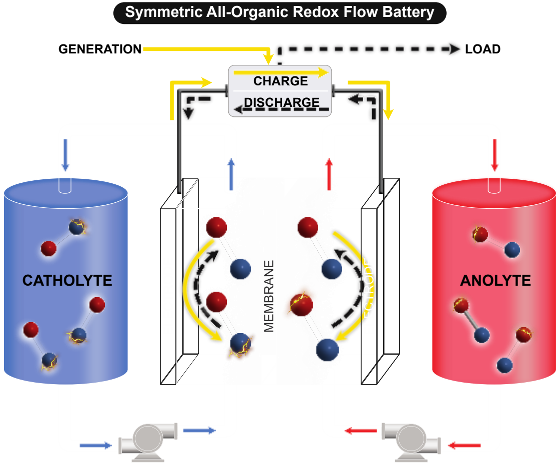
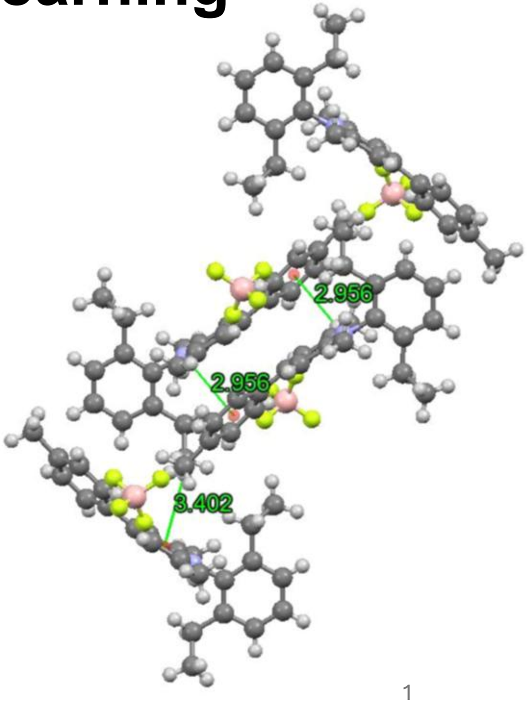
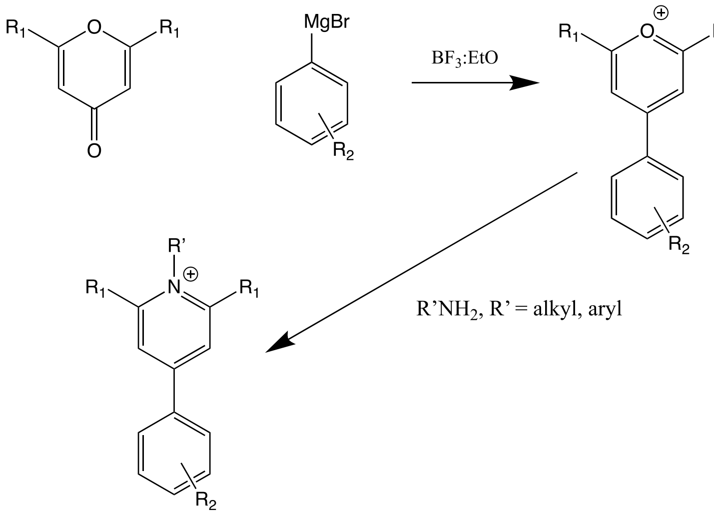
International Flow Battery Forum, Vienna, June 25, 2025





New Pyridinium Anolytes



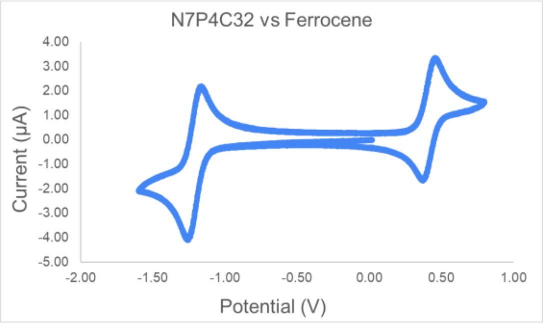
Redox potential
Solubility
} Energy Density

Viscosity
Conductivity
} Energy Efficiency

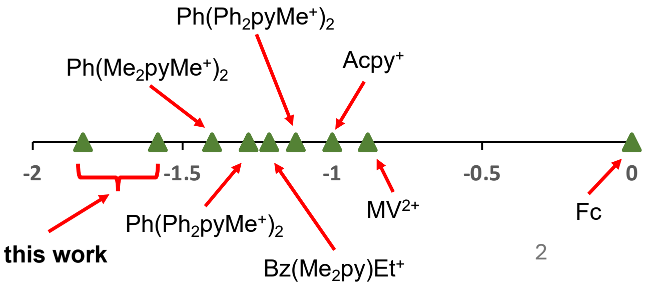
Diffusion coefficient
Electrode kinetics
} Power Density

Radical persistence } Service Life

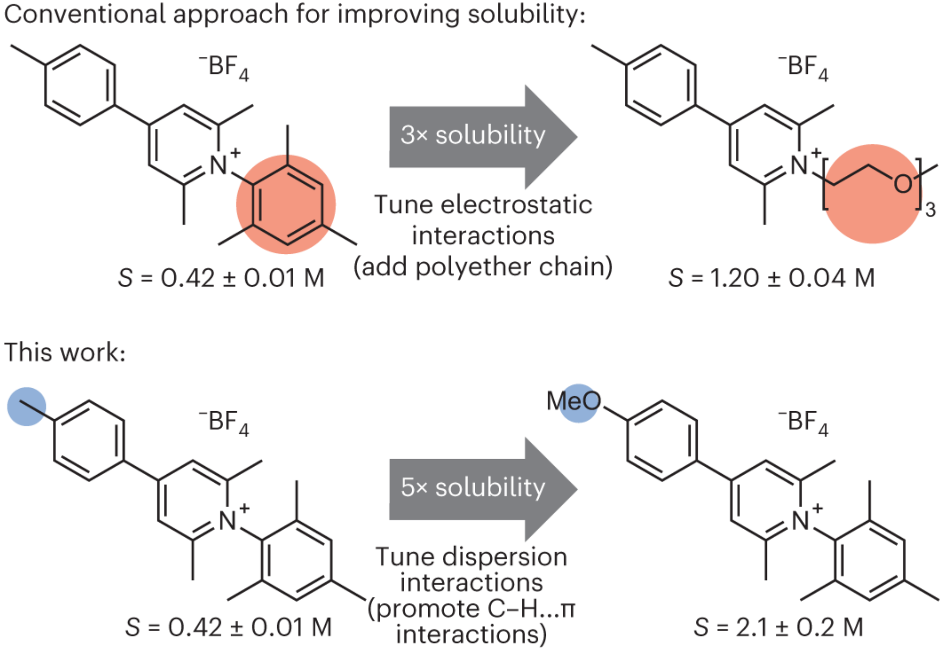
} Commercial Viability

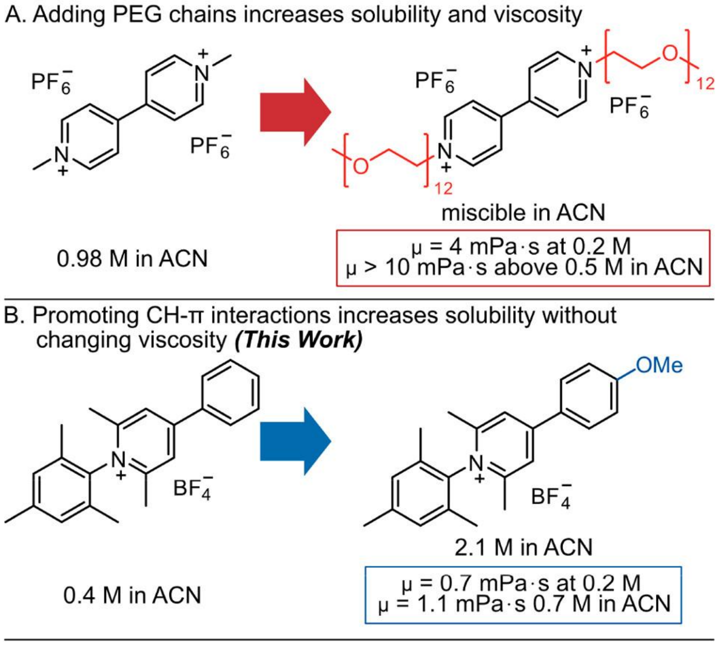


Reduction potentials are nearly 1V lower than MV^{2+} and 0.5V lower than 2,6-Me_2-4-benzoylpyridiniums



Solubility and Viscosity

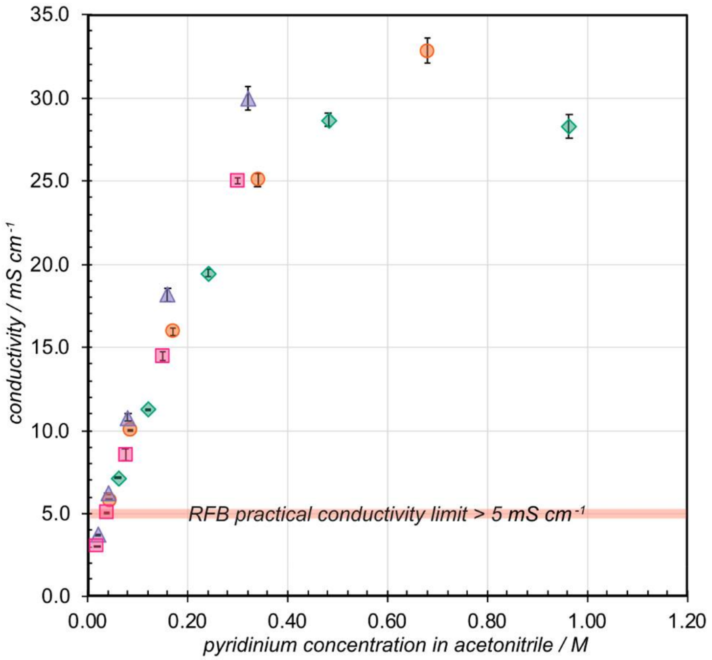


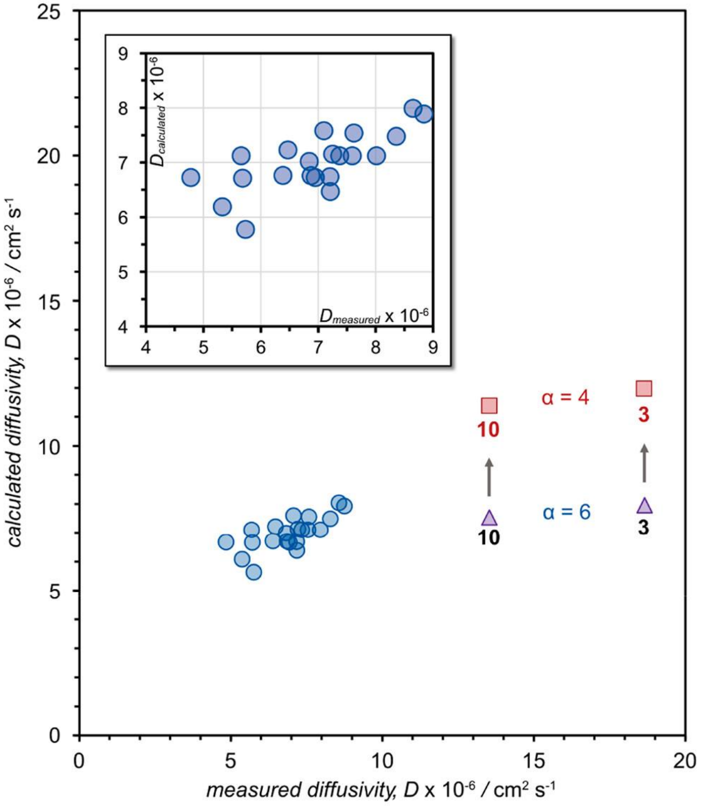


C-H···π interactions disrupt electrostatic interactions between non-aqueous electrolytes to increase solubility
S. Samaroo et al., Nat Chem. 2023 Oct;15(10):1365-1373

Low Viscosity, High Concentration Pyridinium Anolytes for Organic Nonaqueous Redox Flow Batteries
S.Samaroo et al., ACS Appl. Energy Mater. 2024, 7, 18, 7640–7648

Conductivity and Diffusivity





Low Viscosity, High Concentration Pyridinium Anolytes for Organic Nonaqueous Redox Flow Batteries

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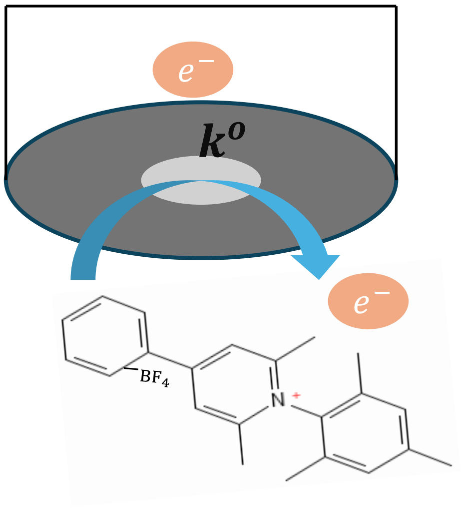
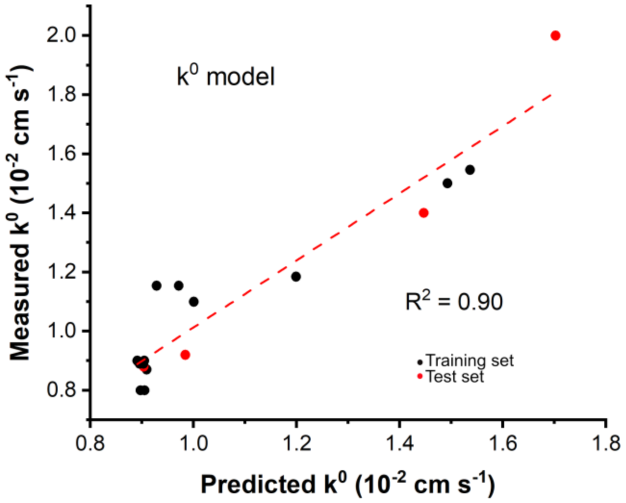
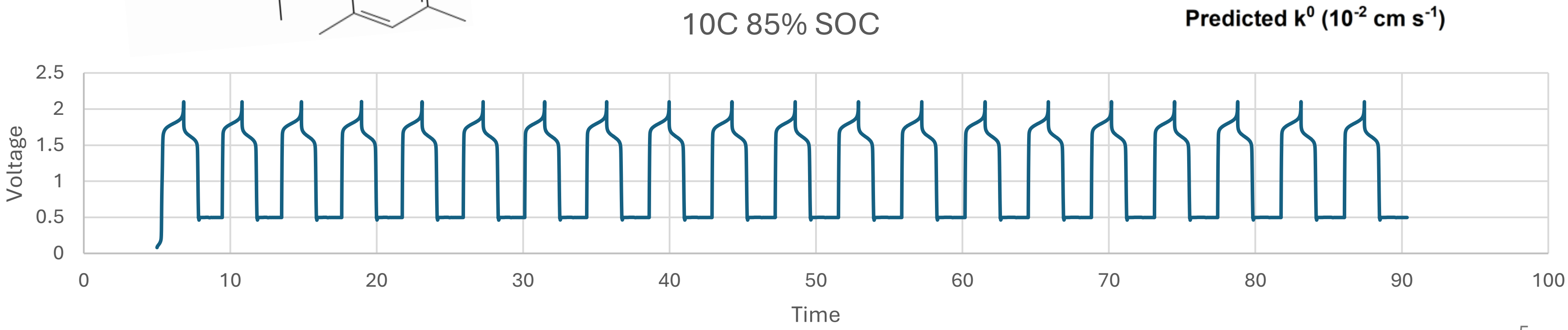
Kinetic Model of Pyridinium Electrochemistry



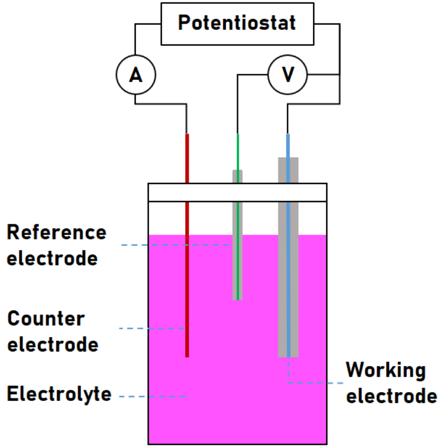
Model describes the electron transfer kinetics of pyridinium molecules at the electrode surface.



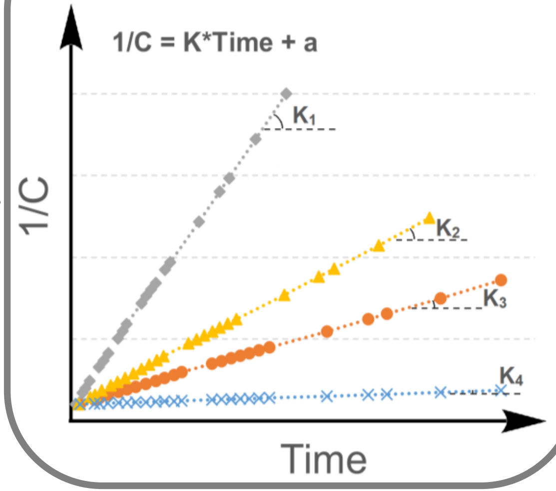


Stability Study

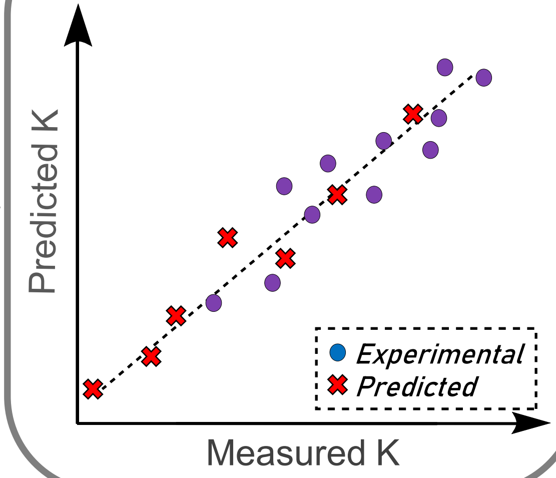
Chronoamperometry



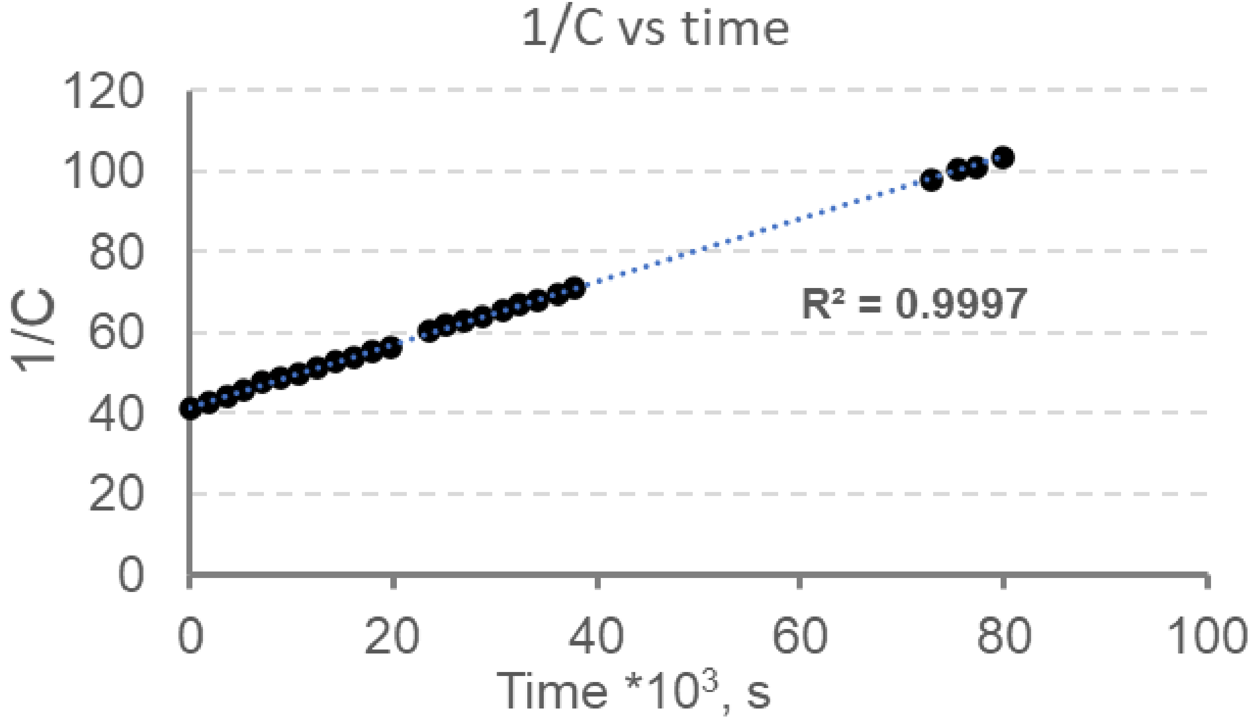
Determining decomposition rates

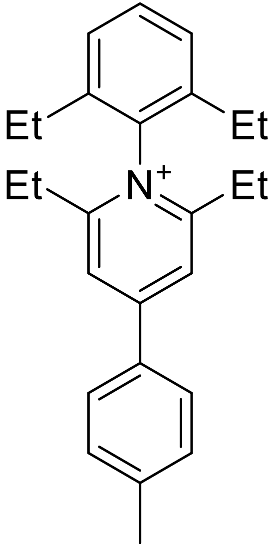


Modeling and predicting stability



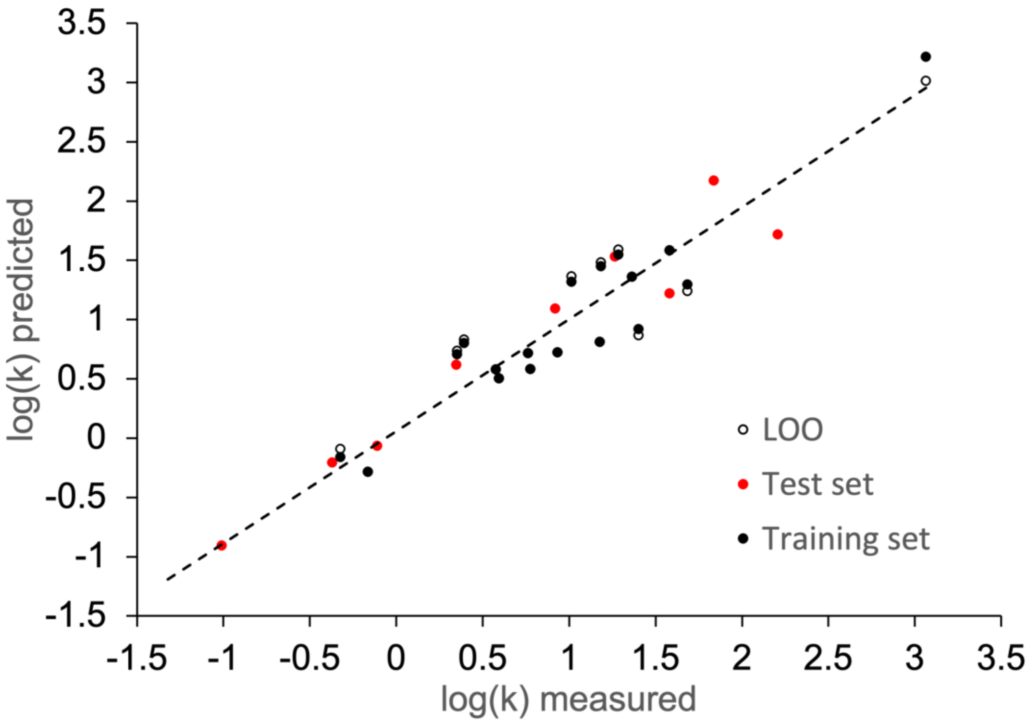
Kinetic Studies



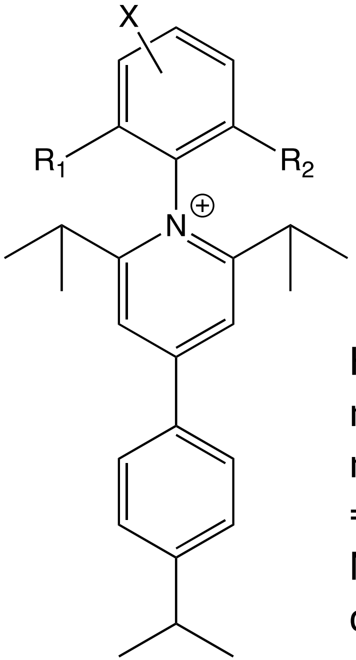


N5P2C2

MLR Stability Model



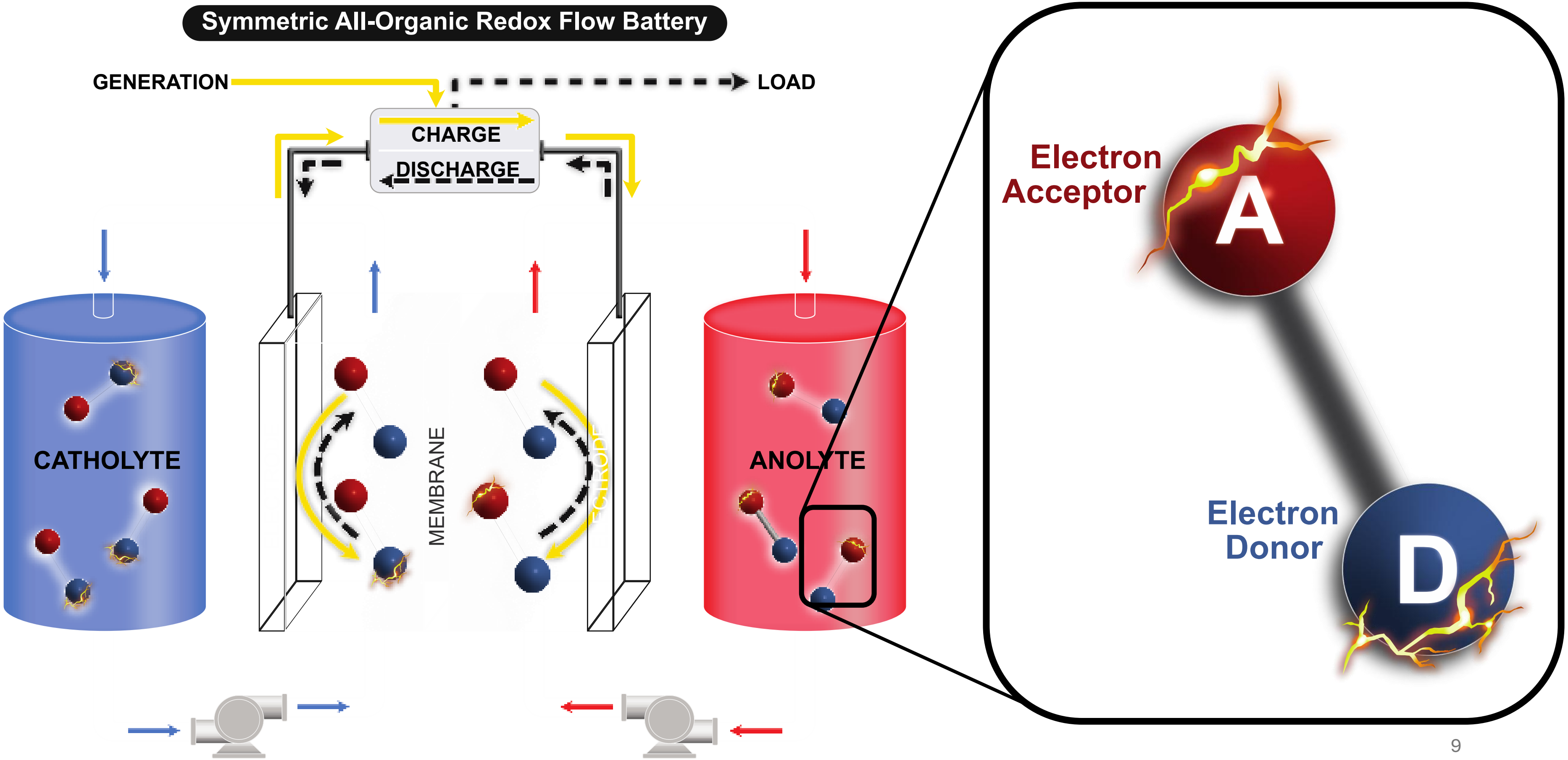
Current Best Performer Subclass



Zeroth order in pyridinium
$k = 9.9*10^{-10}$ M/s

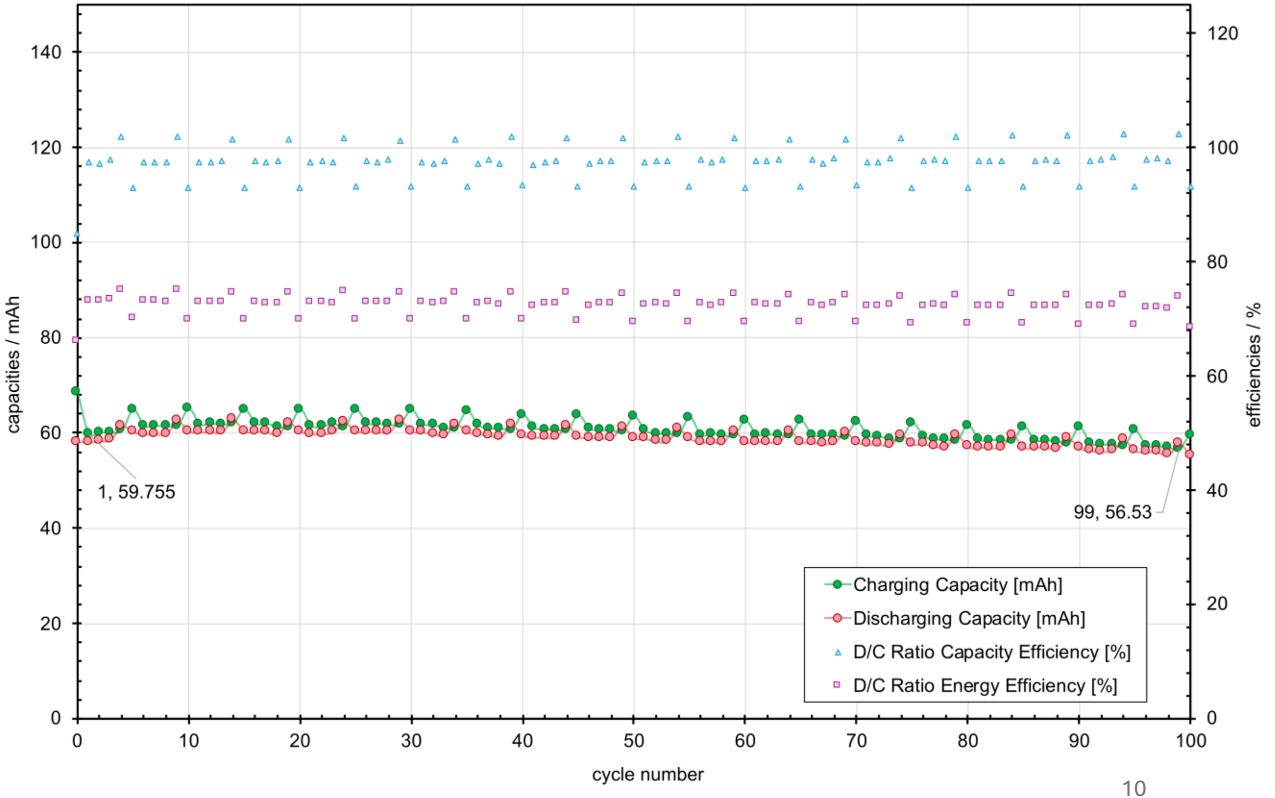
Half-life of 1M radical solution at room temperature = approx. 16 years
No chemical decomposition detected

RFB electrolyte contains linked anolyte and catholyte

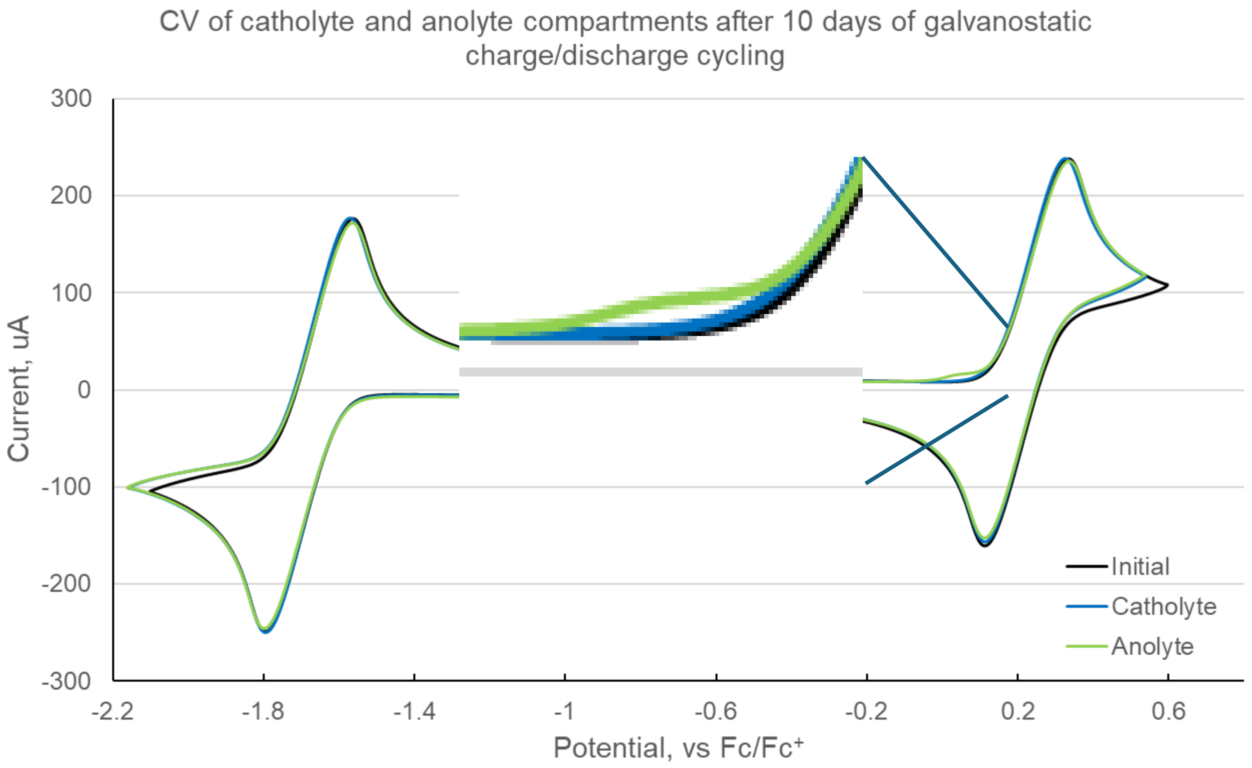


Flow Cell Cycling

Redox Species:	T8
Concentration:	100 mM
Solvent:	PC
Electrolyte:	TEATFSI (500 mM)
Theoretical Capacity:	Approx. 100 mAh
Flow Rate:	400 mL/min
Current Density:	20 mA/cm^2
Electrodes:	Sigracell 4.65 GFD
Membrane:	Celgard (25 um)
Cycling Conditions:	N2 glovebag, room temperature
Capacity Fade:	0.055% per cycle
Coulombic Efficiency:	97.3% +/- 3.0%
Energy Efficiency:	72.2% +/- 1.7%



RFB Electrolyte Post-cycling Analysis



Static Scribner cell

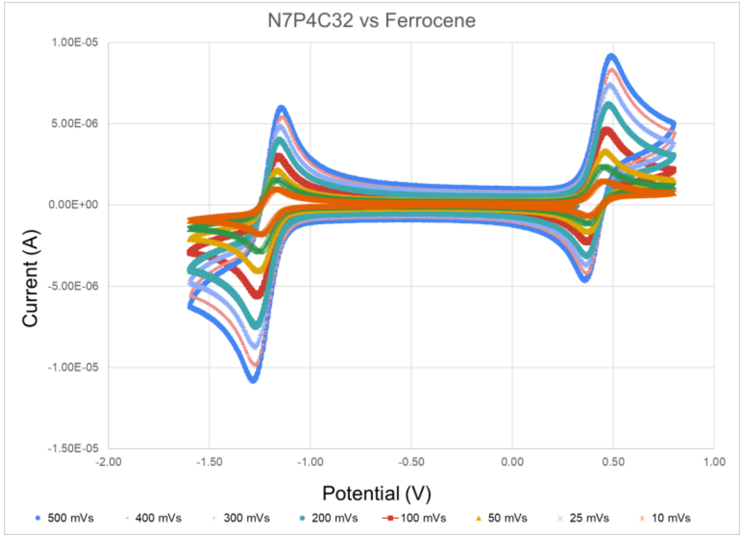
- 100mM working electrolyte
- 0.5M supporting electrolyte
- 2mA/cm^2 charge/discharge current

Take-Home Message

Redox active organics offer enormous molecular design freedom

Machine Learning models have guided substantial improvements in:

- Solubility
- Diffusion coefficients
- Viscosity
- Electrode kinetics
- Radical persistence



Linked Catholyte/Anolyte systems show good cycle and calendar life, but some issues remain

MICHIGAN STATE
UNIVERSITY

Acknowledgments

JOLT
ENERGY STORAGE TECHNOLOGIES

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

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LAKESHORE ADVANTAGE

cfhz community foundation Holland/Zeeland Area

CHAIN REACTION INNOVATIONS
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