Electrochemical Energy Storage through Ligand-Based Charge Manipulation

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Davidson College
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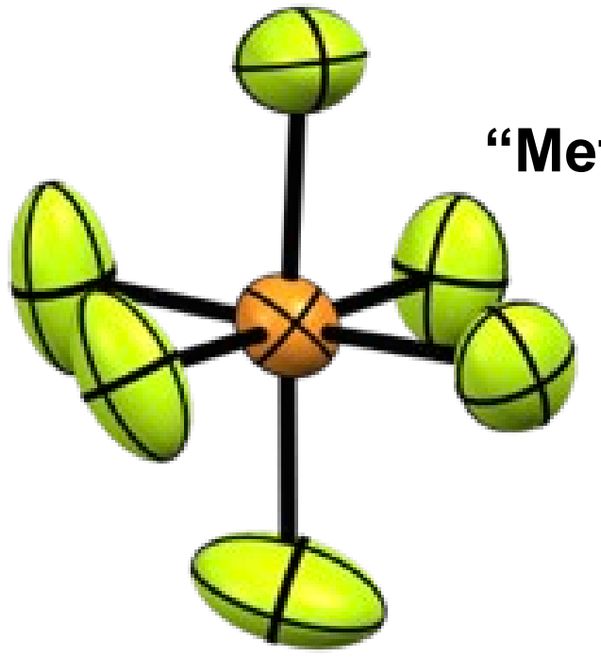
DAVIDSON

Project Overview: Improvement of Battery Charge* Management

Molecular species have an important part to play in battery science.

Guiding Principles:

- **Replacing heavy metals with cheaper main group elements**
- **Using organics/ligands to store charge**



“Metal Complex”

Current Applications and Projects:

- **New Electrolyte Development for RFB**
- **Redox Shuttles for Overcharge Protection**
- **Redox Shuttles to Enhance Charge Mobility**

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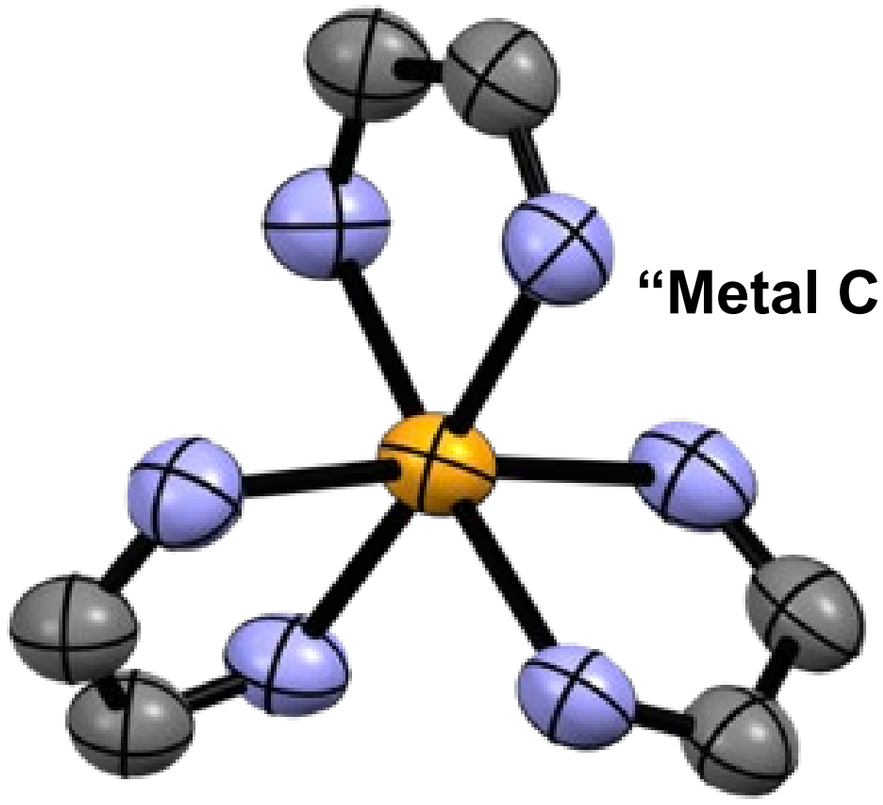

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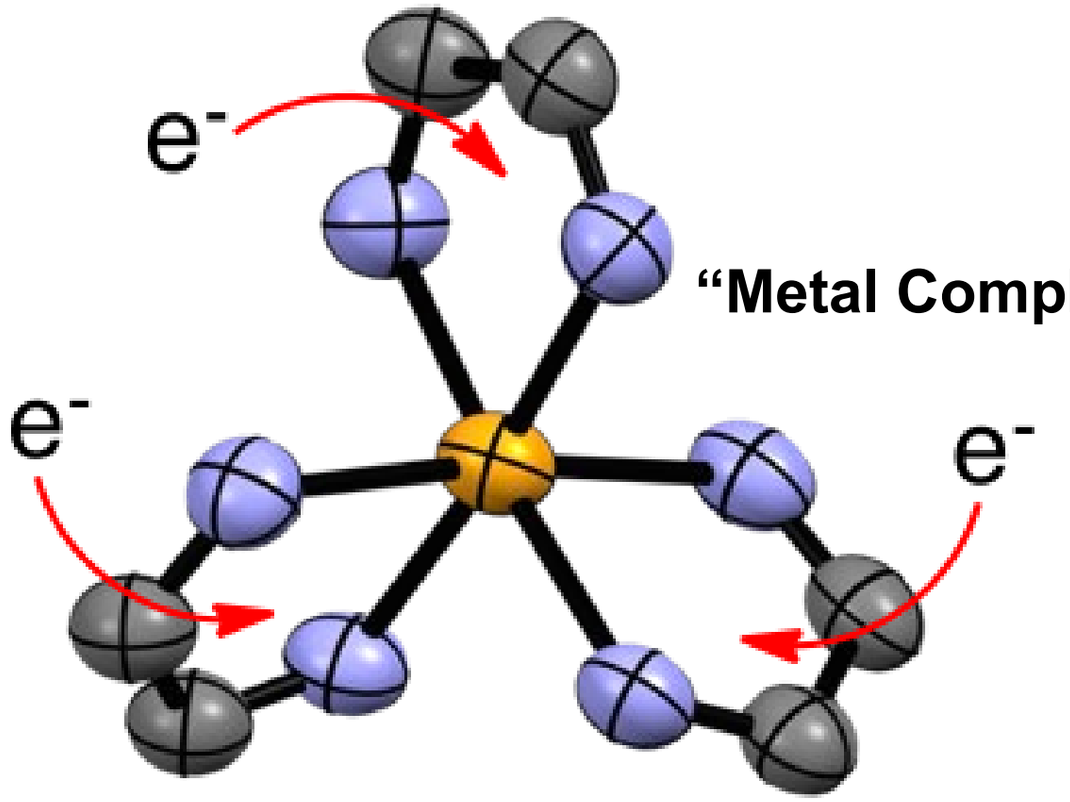

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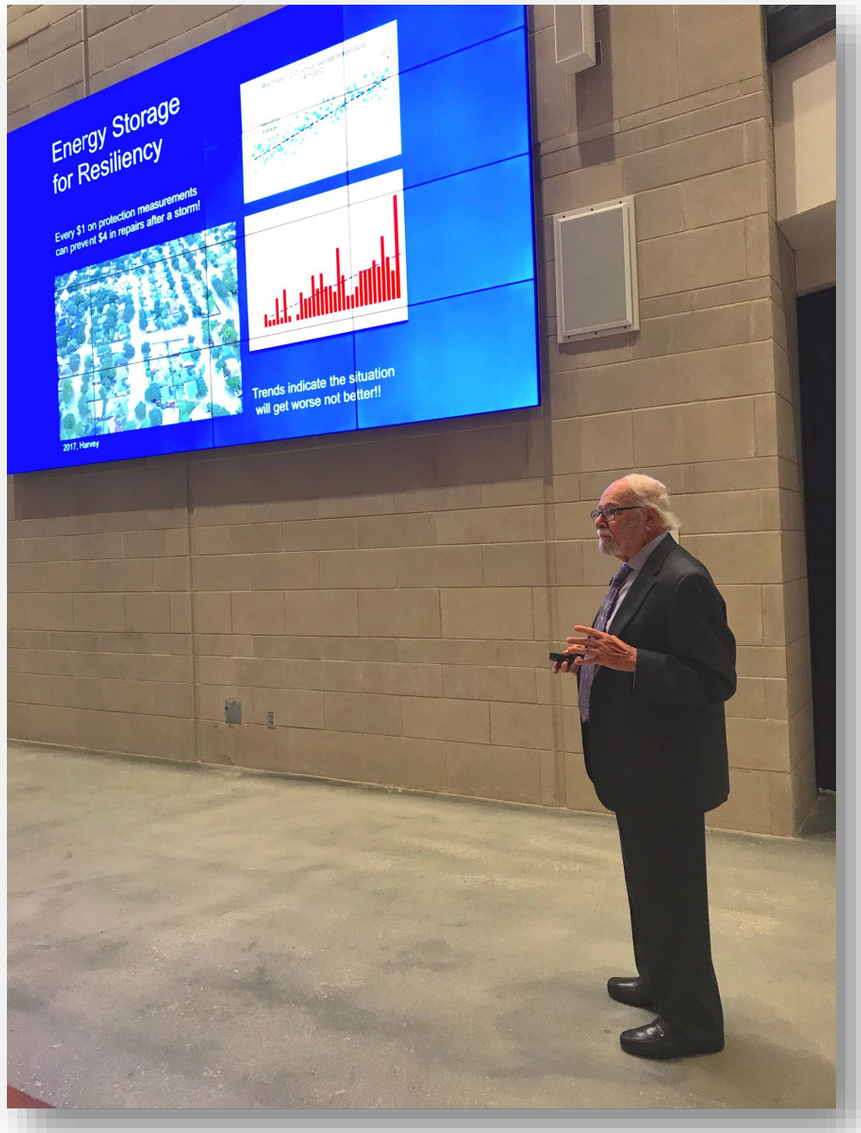
People to Thank

Undergraduate Researchers
Kaycee Gass (‘17)
Allison Hunt (‘17)
Cole Cuthbertson (‘18)
Lucas Kane (‘18)
Nathan Rudman (‘18)
Jennie Goodell (‘19)
Nick Kennedy (‘19)
Claudia Hernandez (‘20)
David Thole (‘21)
Jay Nicoleau (‘21)

Collaborators
Travis Anderson (SNL)
Christopher Bejger (UNC, Charlotte)
Susan Odom (University of Kentucky)
Neil Tomson (University of Pennsylvania)

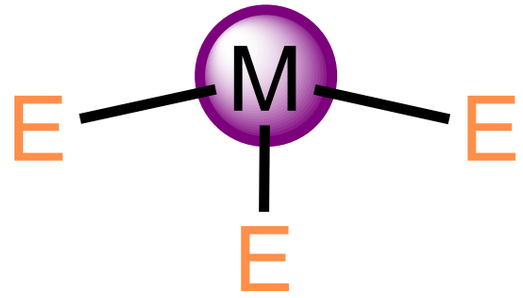
Support
Dr. Imre Gyuk
DOE-OE Program
Babu Chalamala (SNL)
Travis Anderson (SNL)
Davidson College & DRI Program
Department of Chemistry

Dr. Gyuk visiting Davidson last Fall



Electrolyte Design

Electrolyte Design



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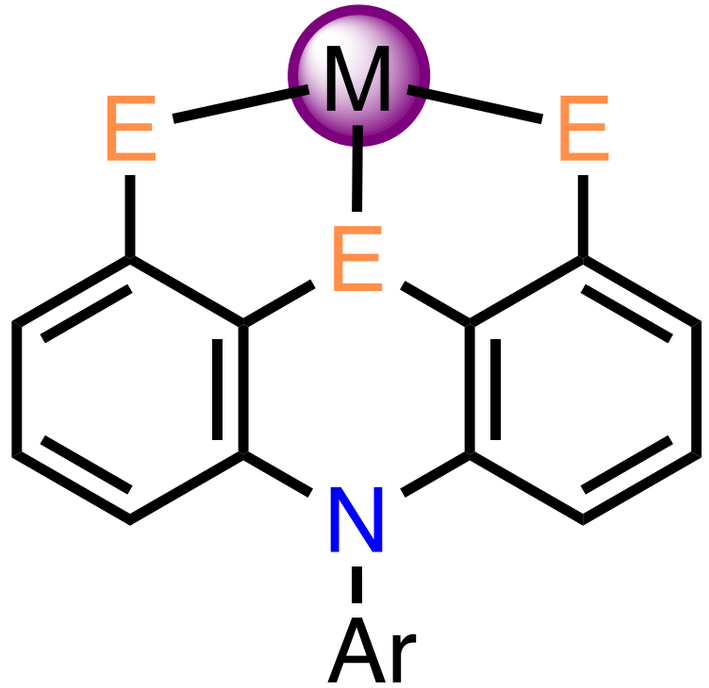
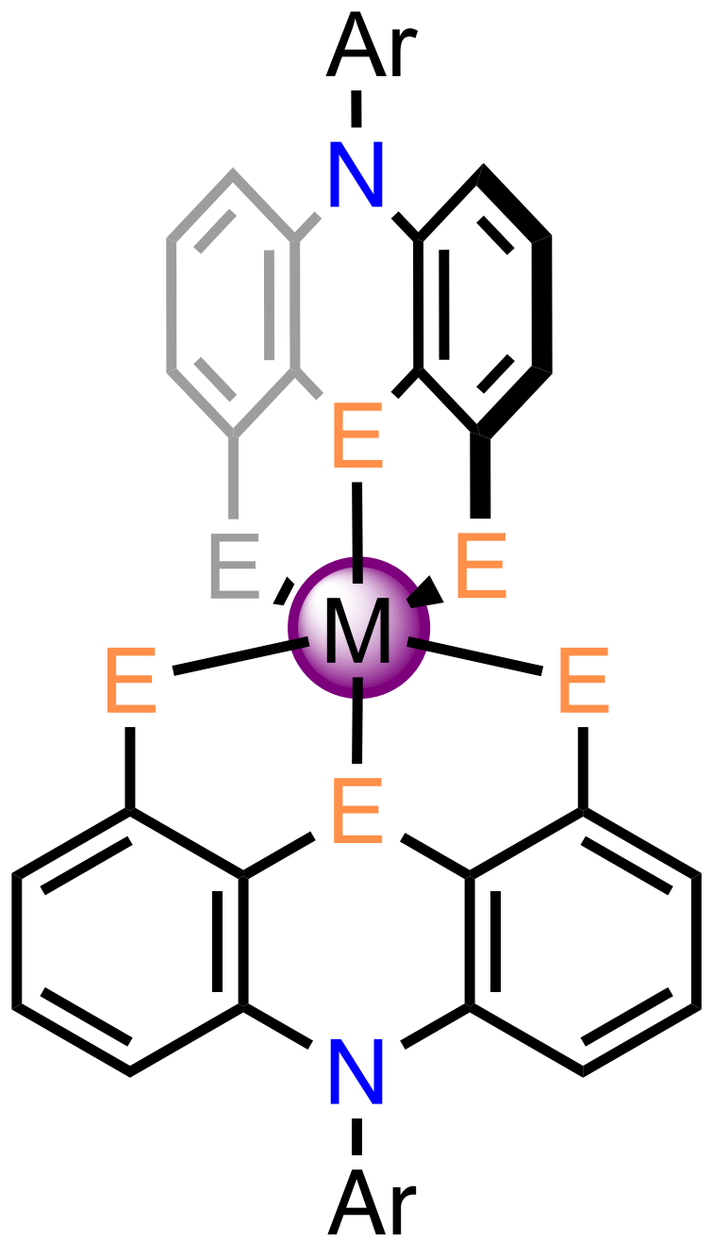
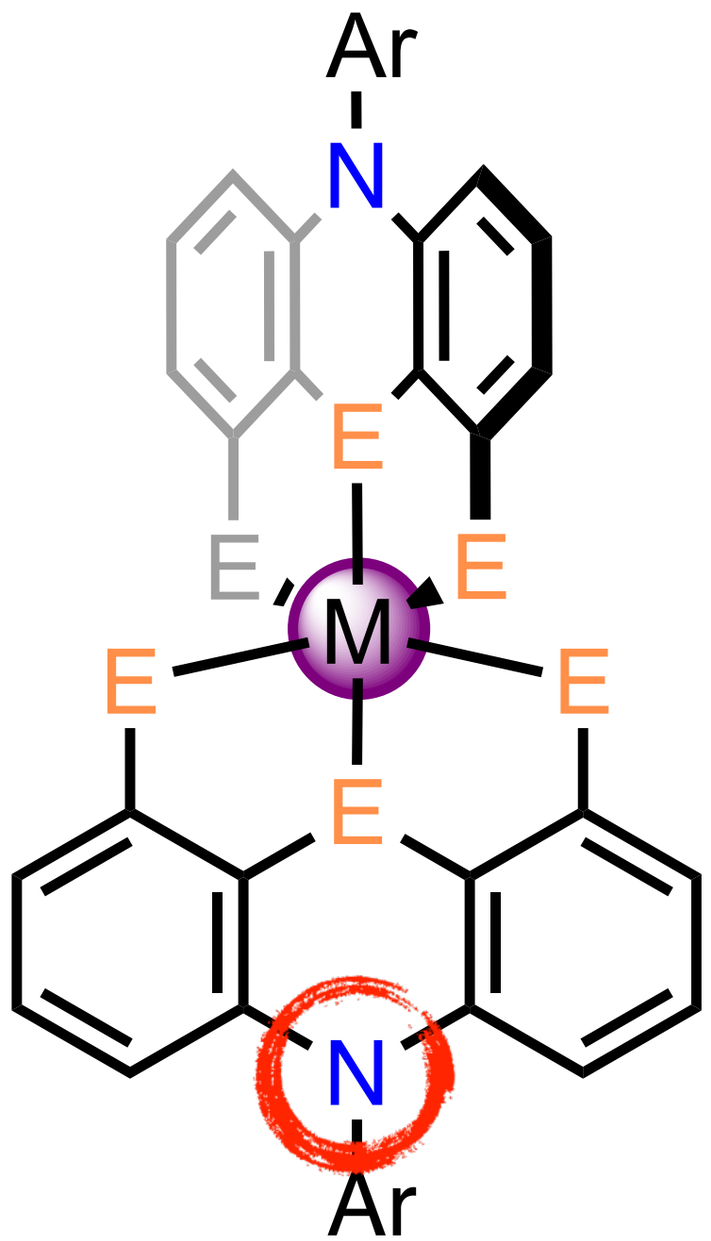


Electrolyte Design



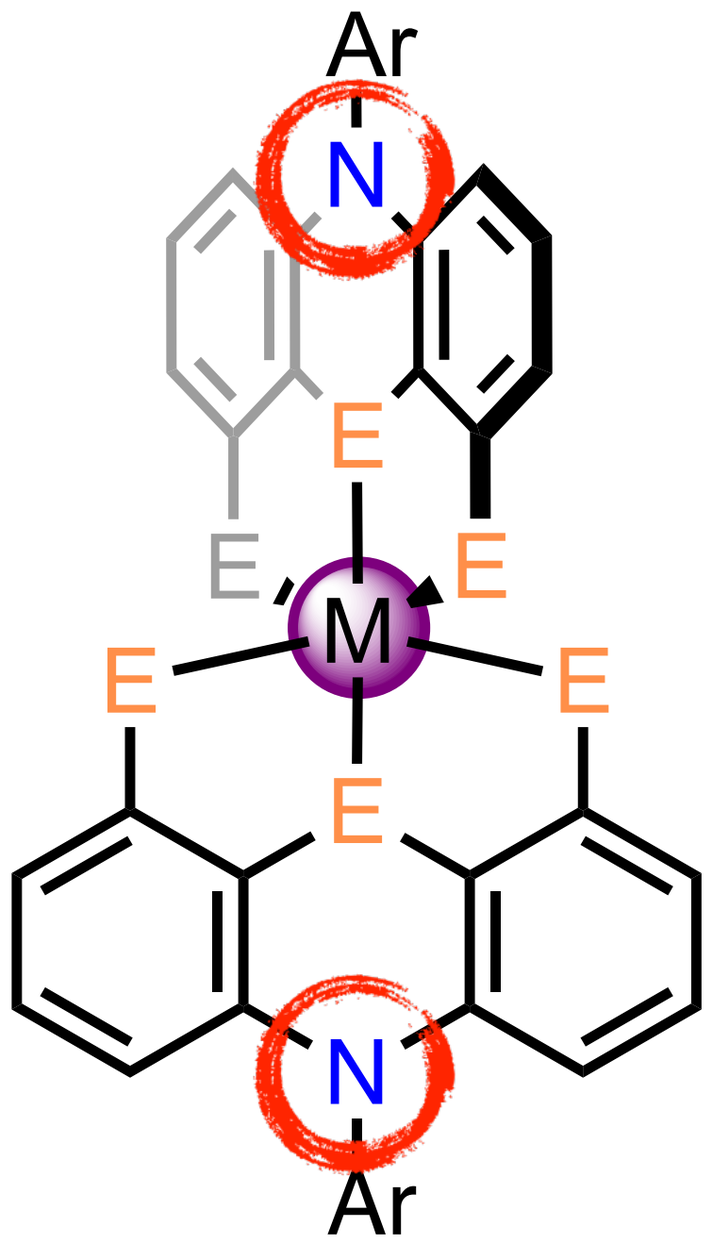
Electrolyte Design



Based on molecular modeling, this is the charge center of the ligand

Electrolyte Design

Two charge centers…



Electrolyte Design

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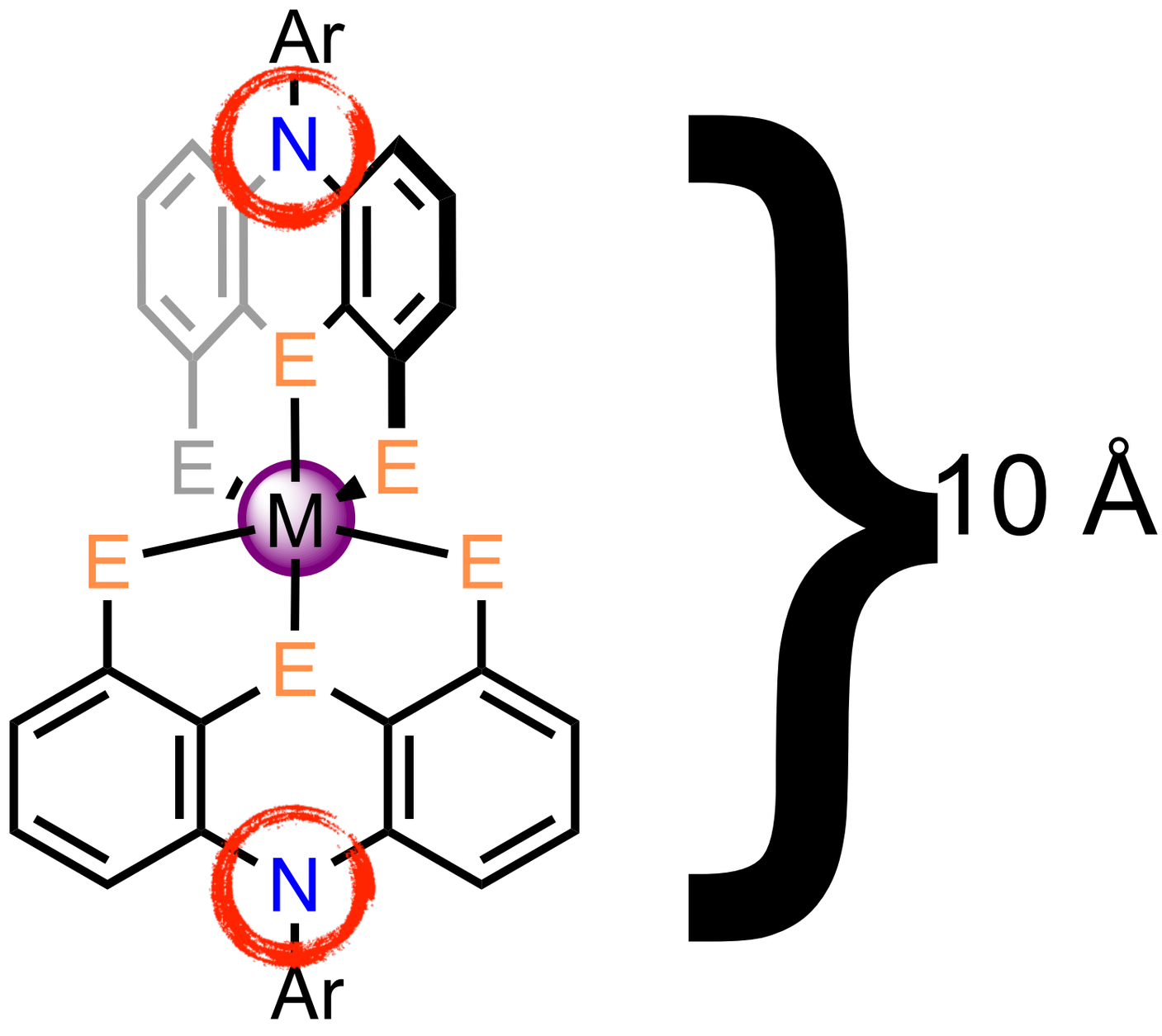
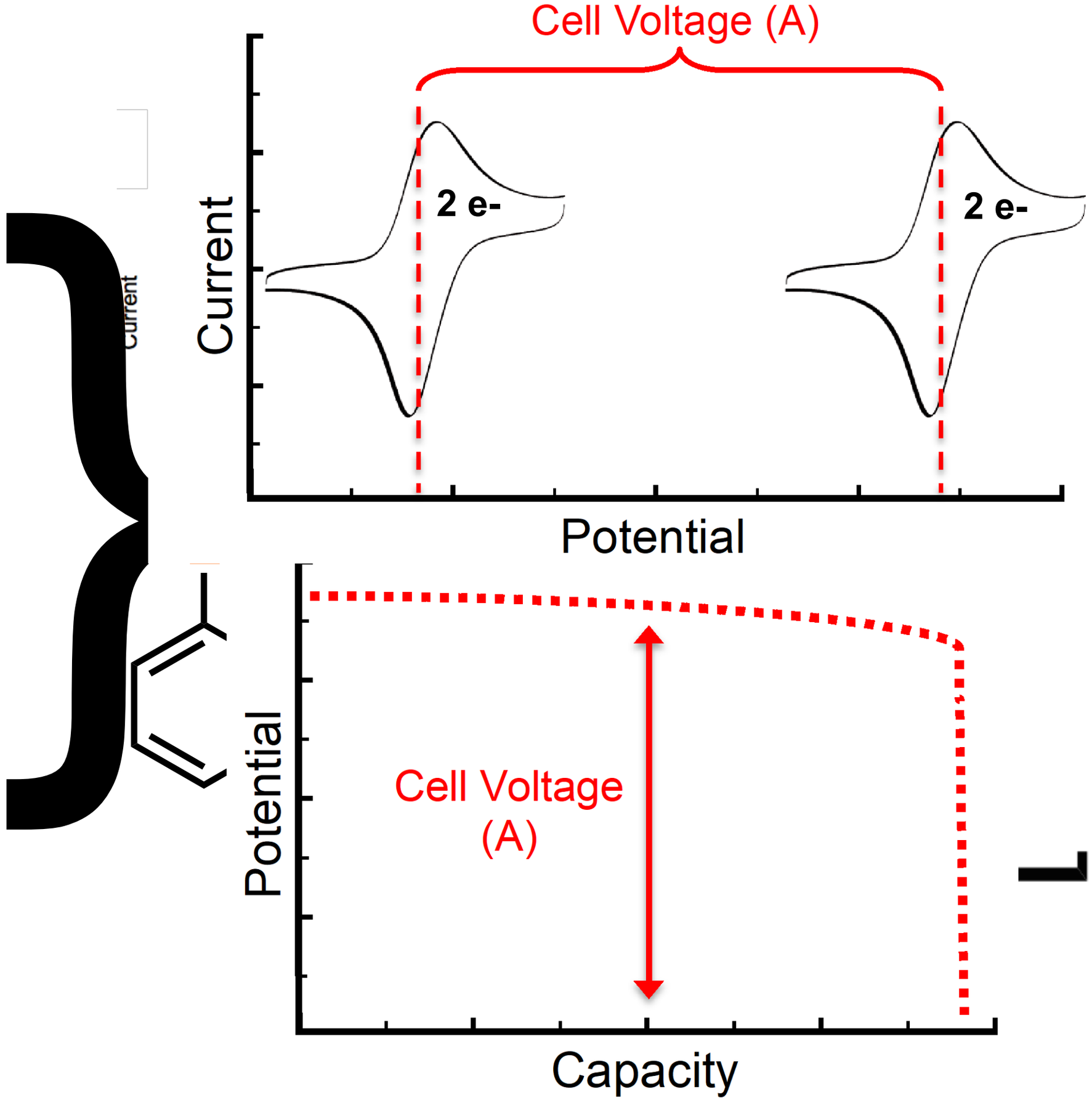
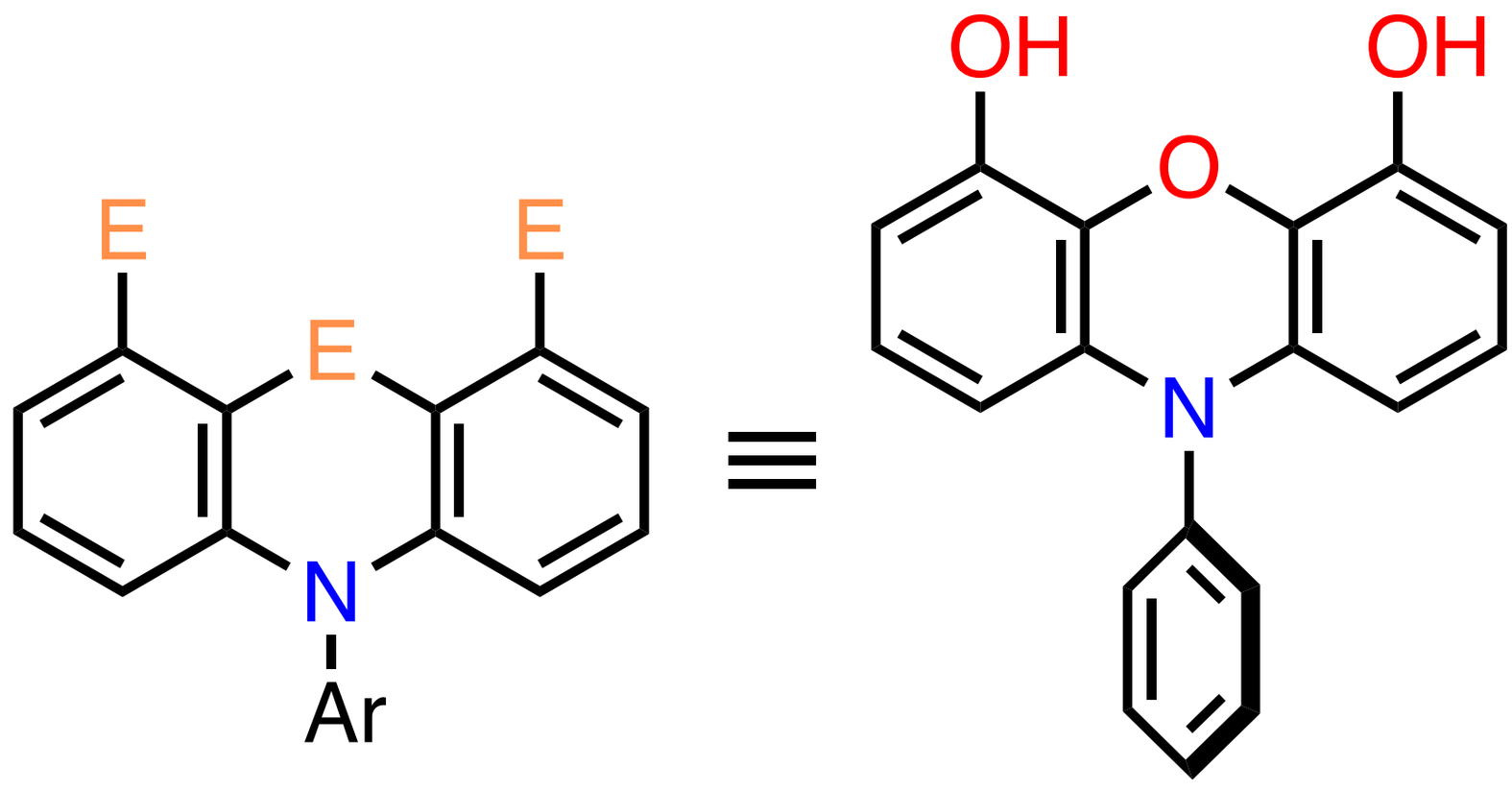
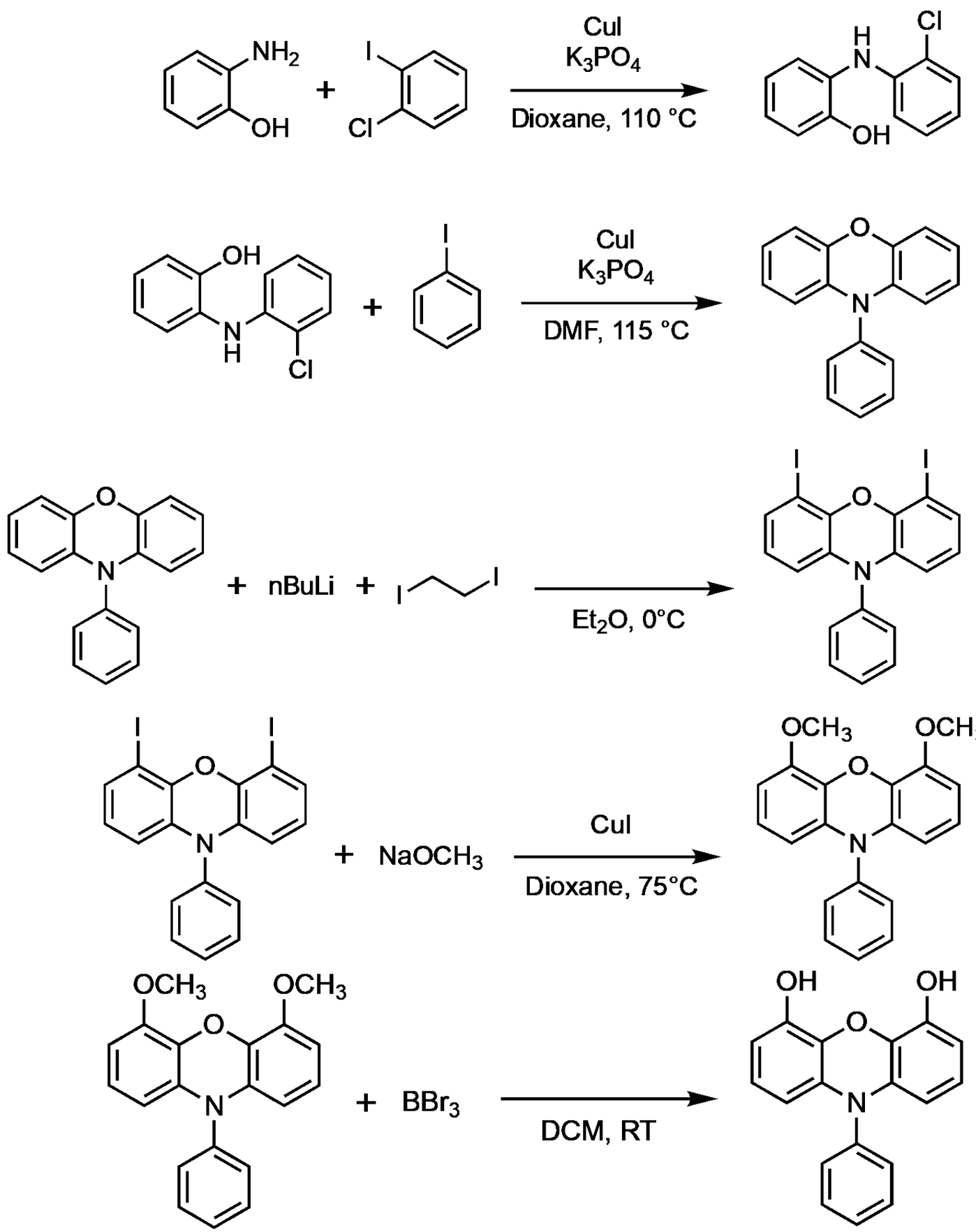


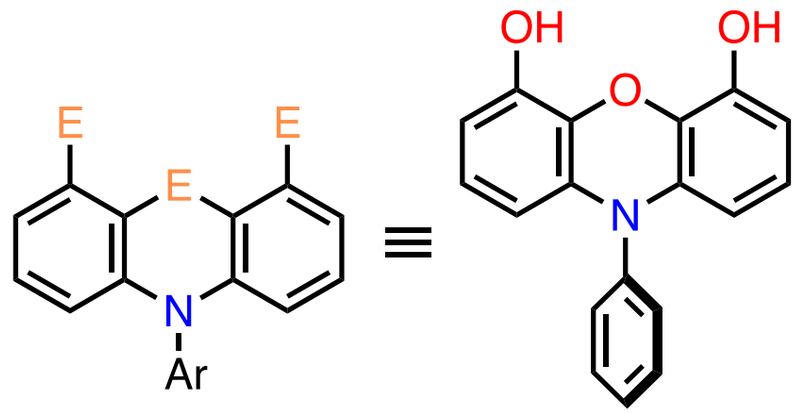
…displaced from one another by a “large” distance.


Current
Cell Voltage (A)
2 e-
2 e-
Potential
Potential
Cell Voltage
(A)
Capacity



Target Compound



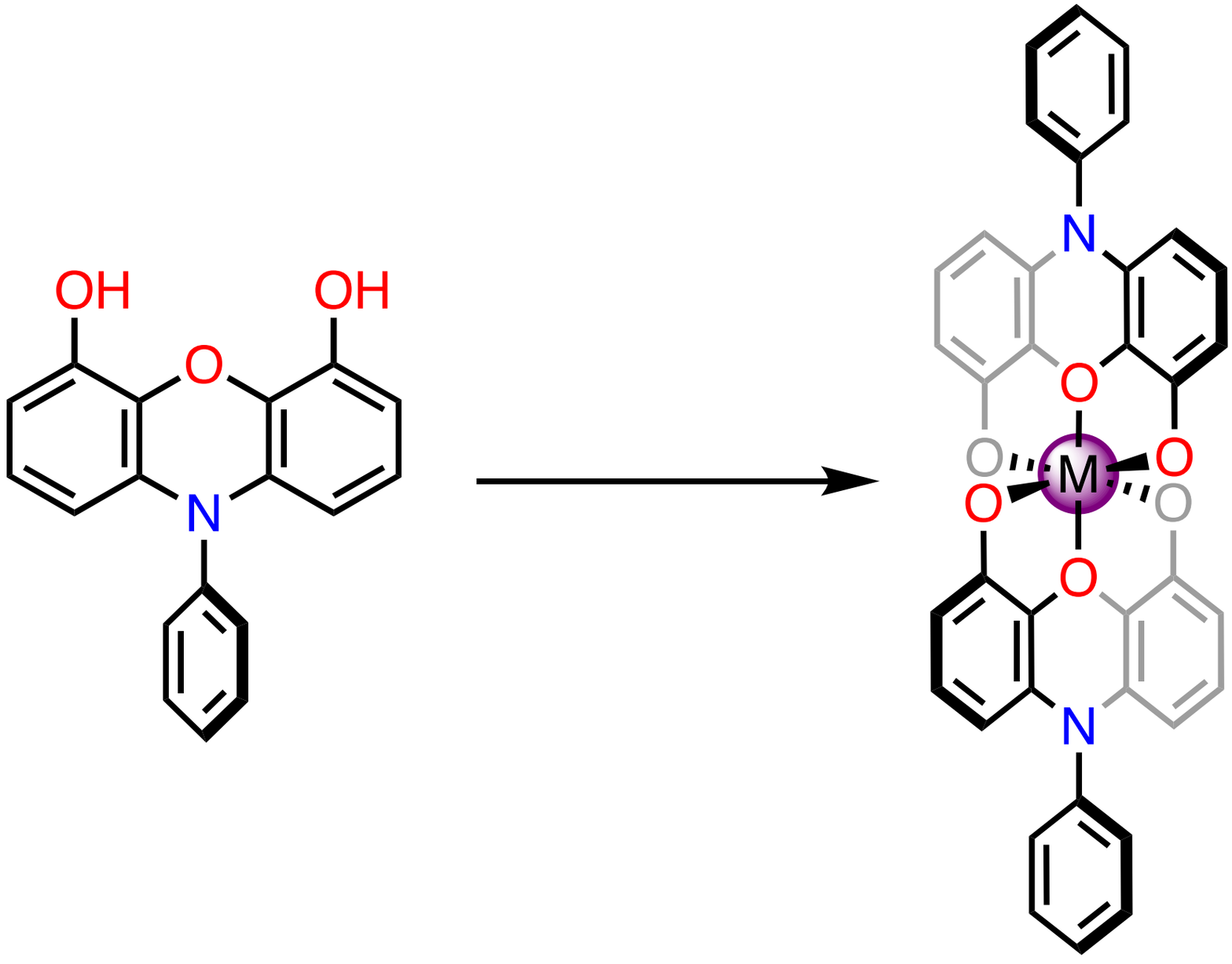


Full procedure:
31% yield, 5 grams

Performed by undergraduate students

Claudia Hernandez (‘20)
David Thole (‘21)

Next Steps



Metal = Titanium, Silicon, Aluminum

1) Synthesize examples of Ti, Si, and Al compounds
2) Analyze redox behavior
3) Publish paper on these results

Redox Shuttles for Overcharge Protection

Susan Odom (Kentucky)
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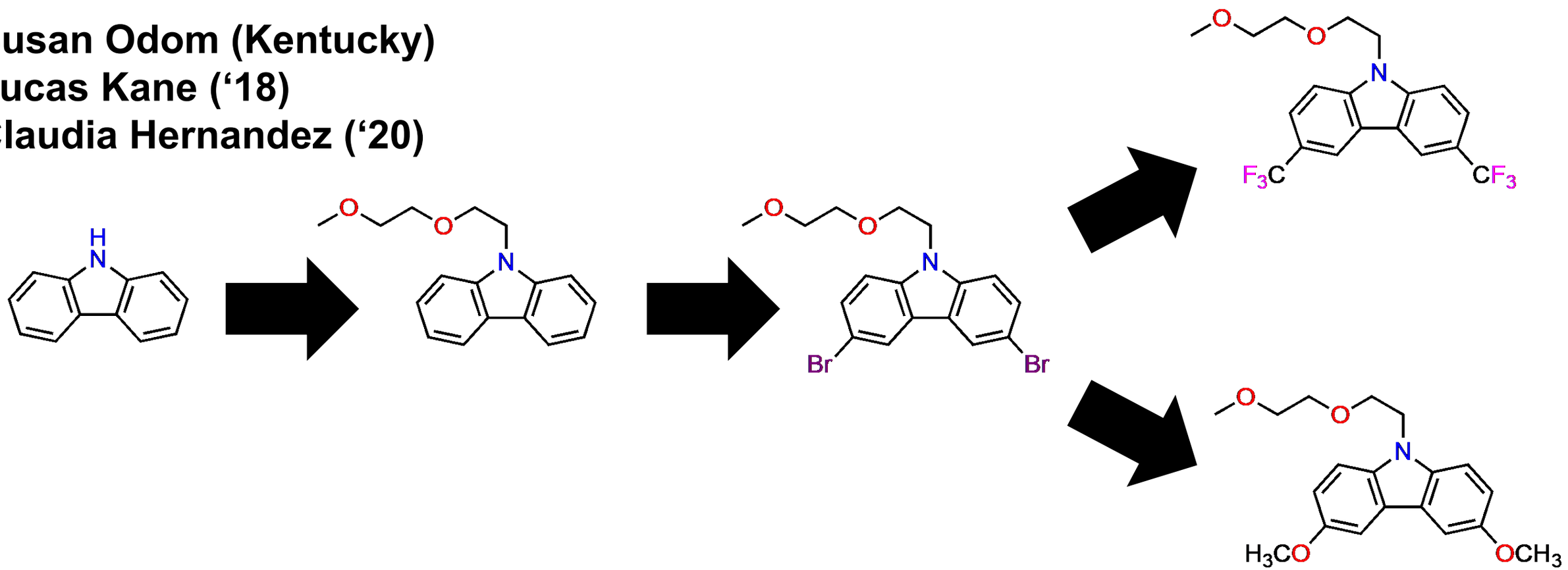

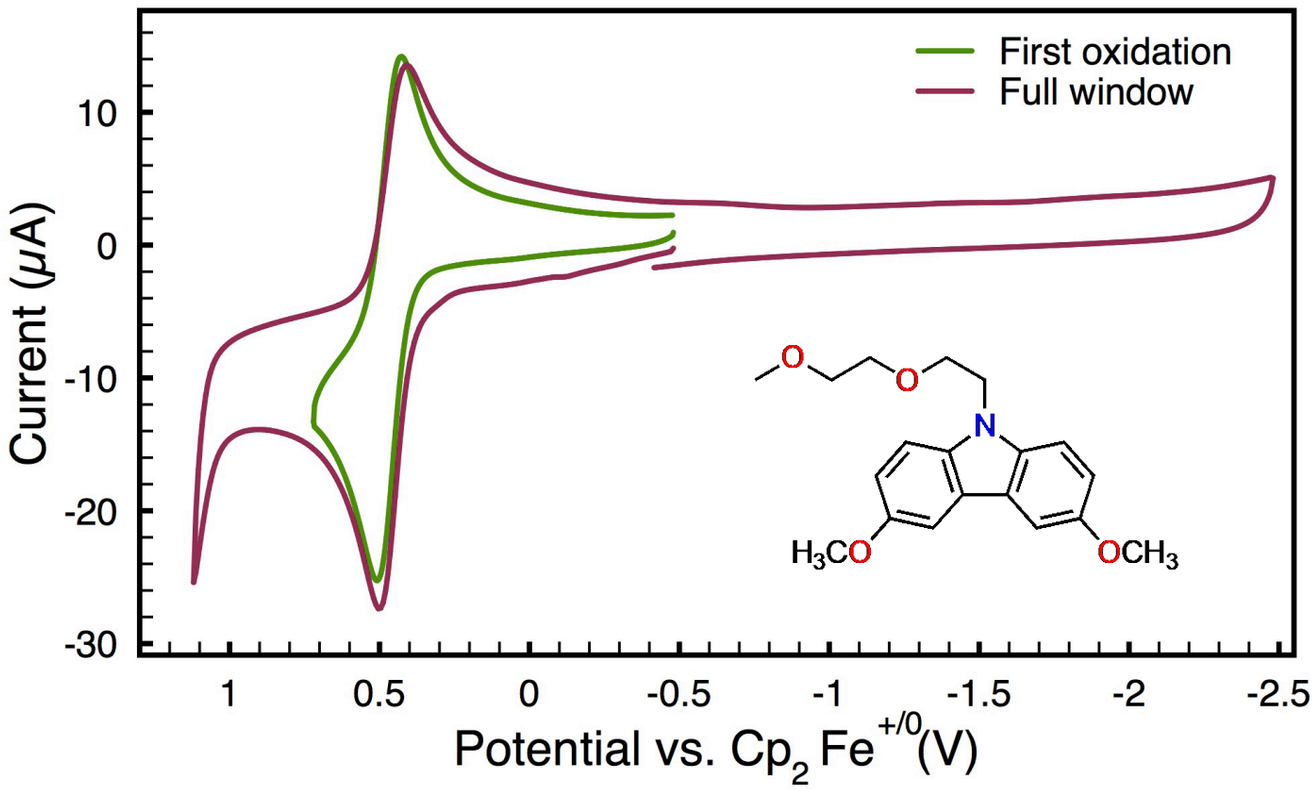

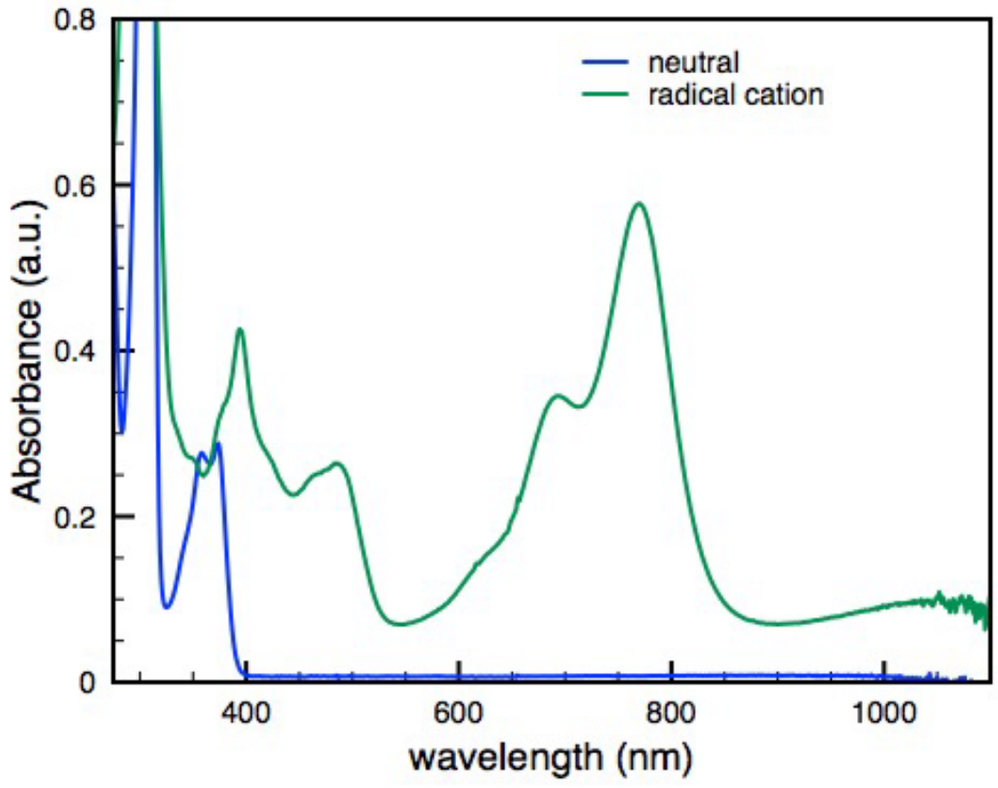

Electrochemically generated radical cation in DCM

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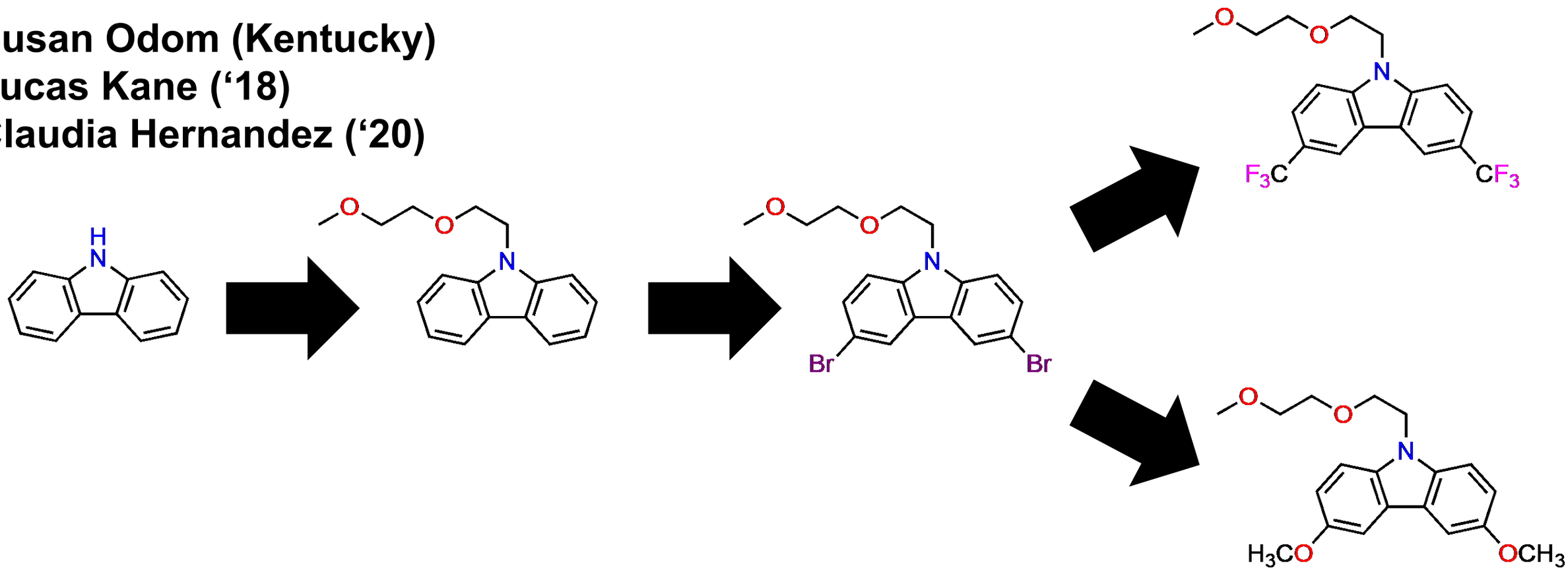
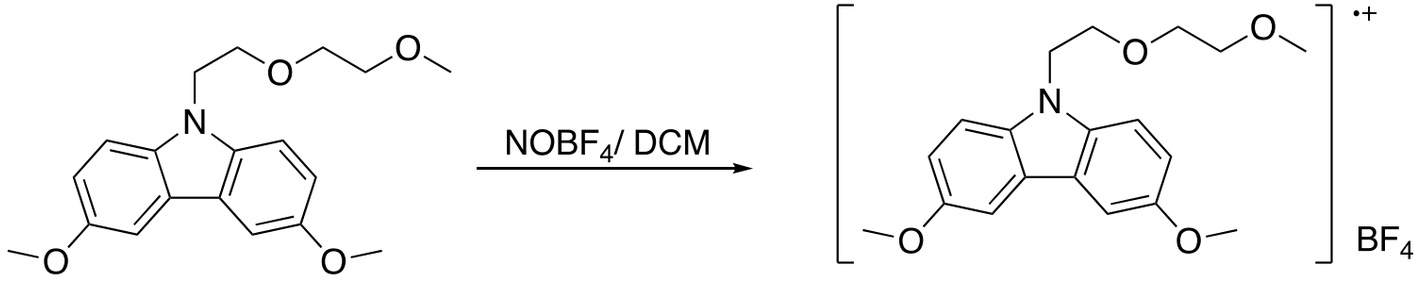
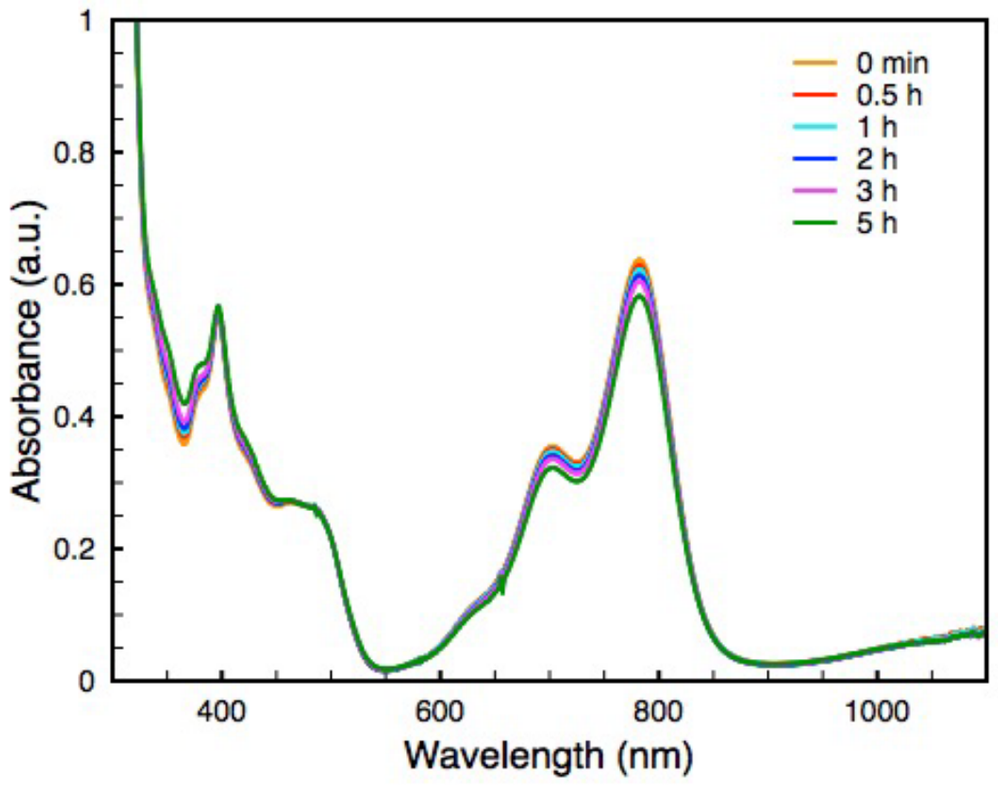




Measuring lifetime/persistence and solubility of active species



Chemically generated radical cation in DCM

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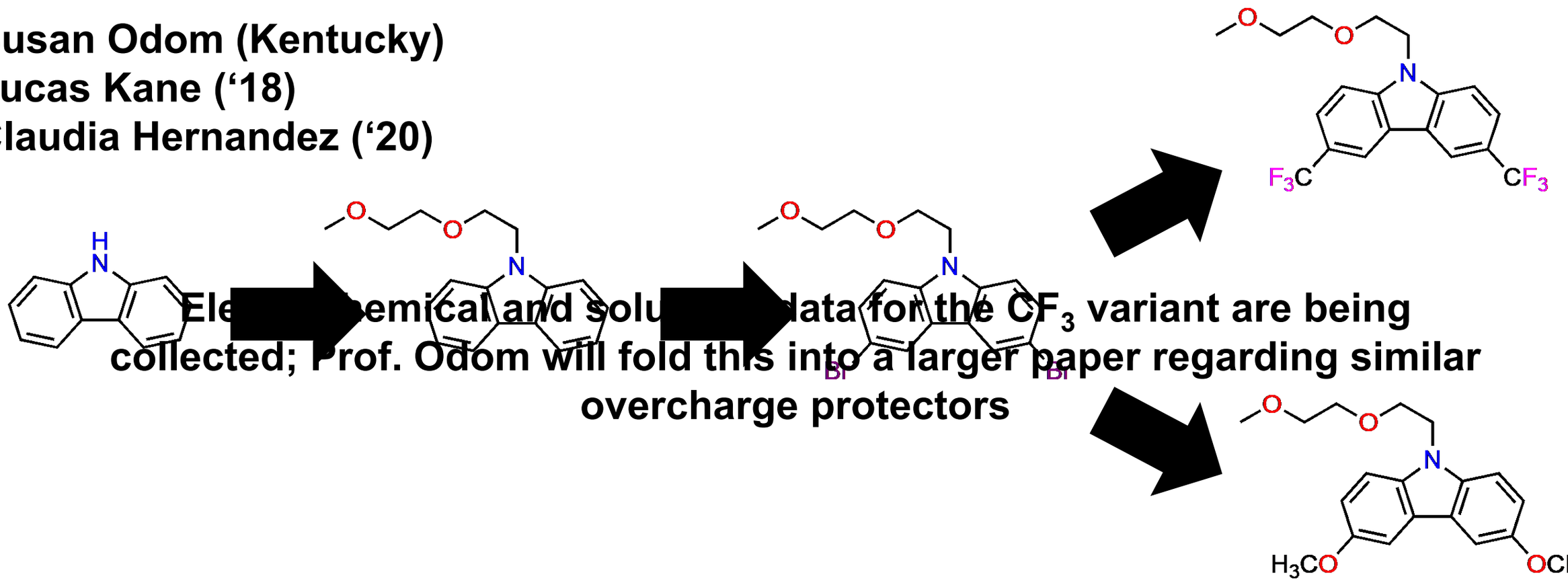
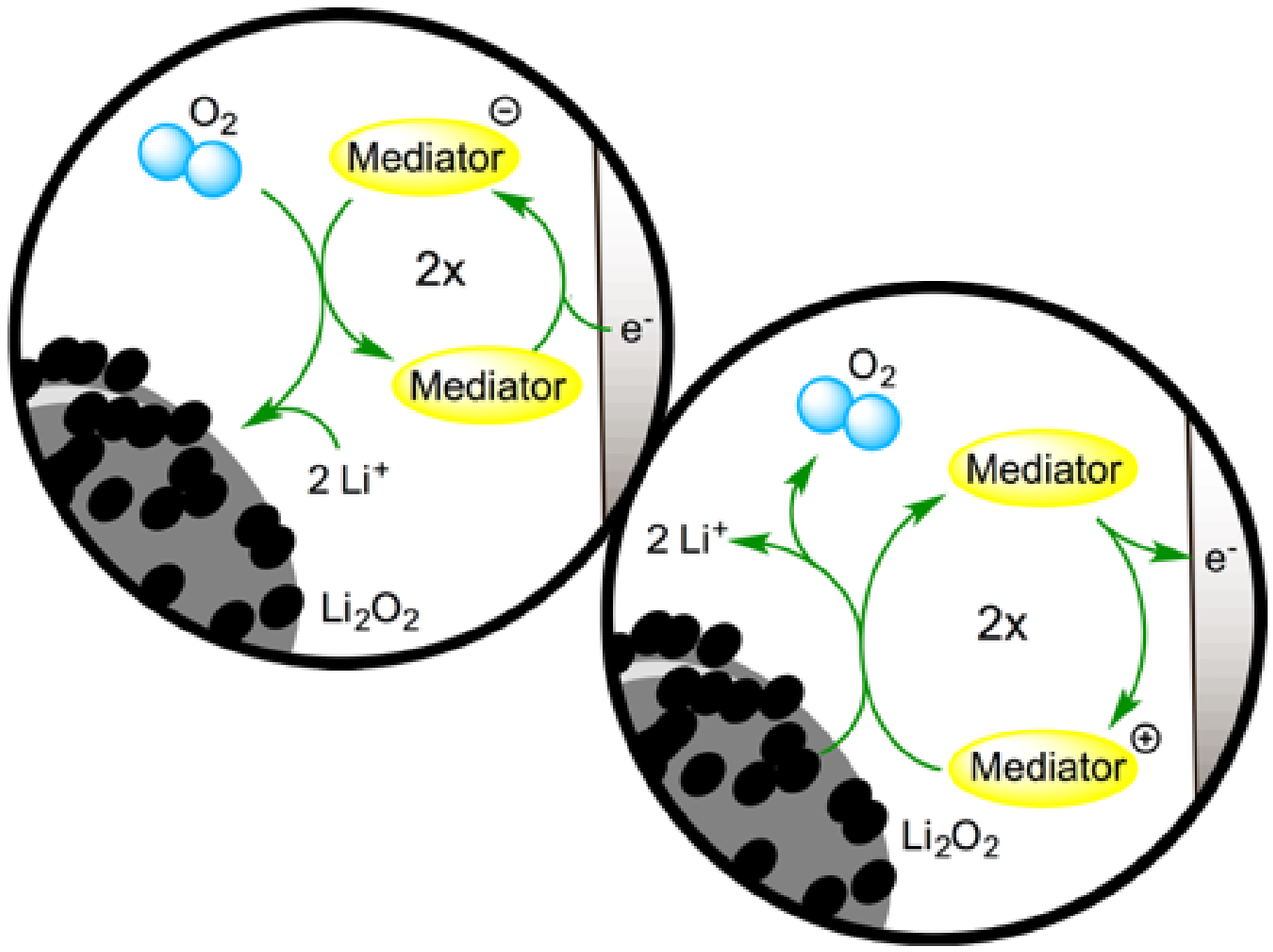
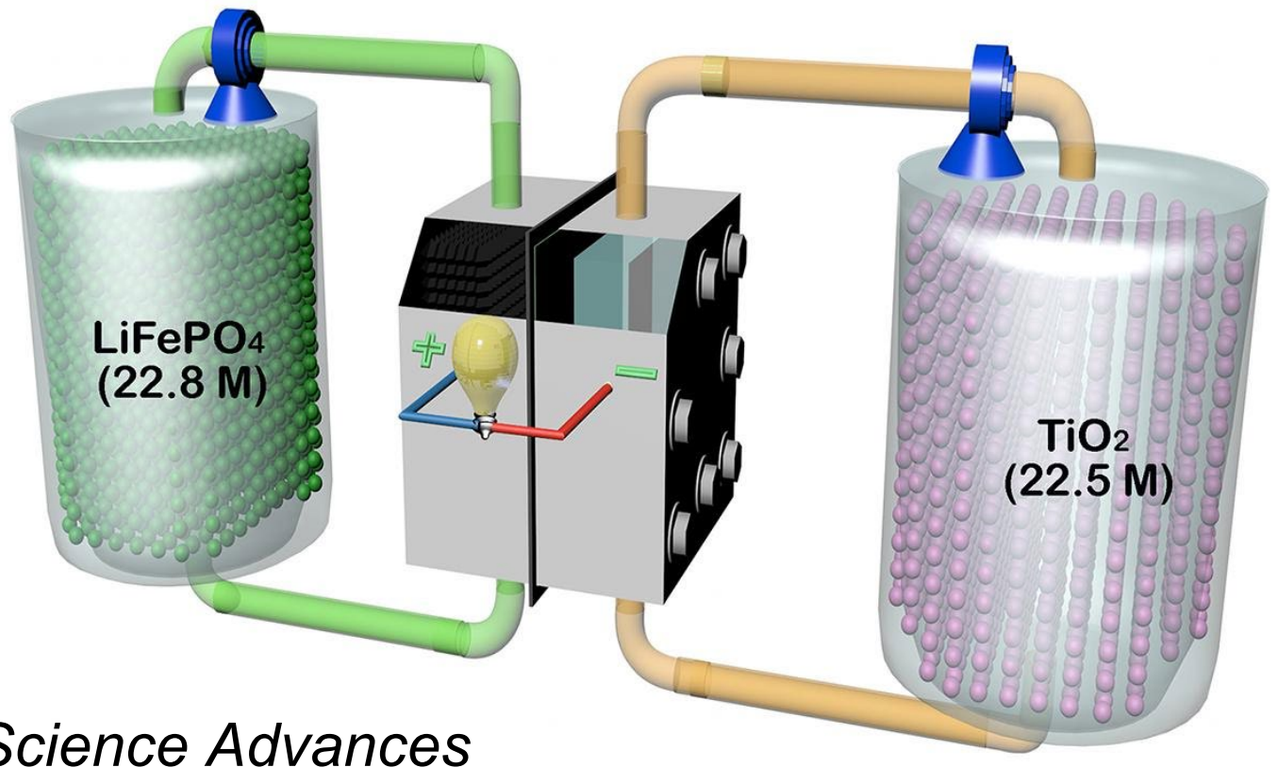


Electrochemical and solubility data for the CF_3 variant are being collected; Prof. Odom will fold this into a larger paper regarding similar overcharge protectors

Redox Shuttles to Enhance Charge Mobility

Next-Gen Unconventional Redox Pairs





RFB with Solid "Electrolyte"

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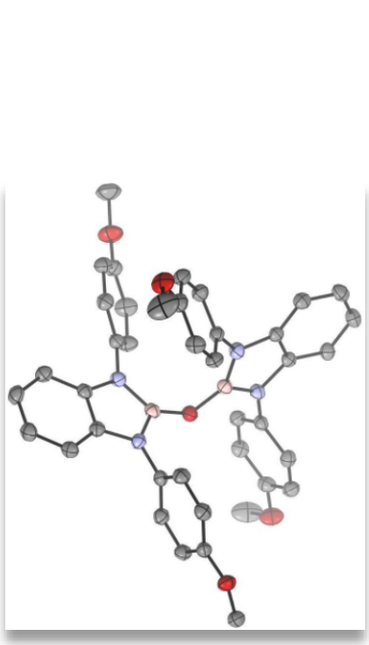
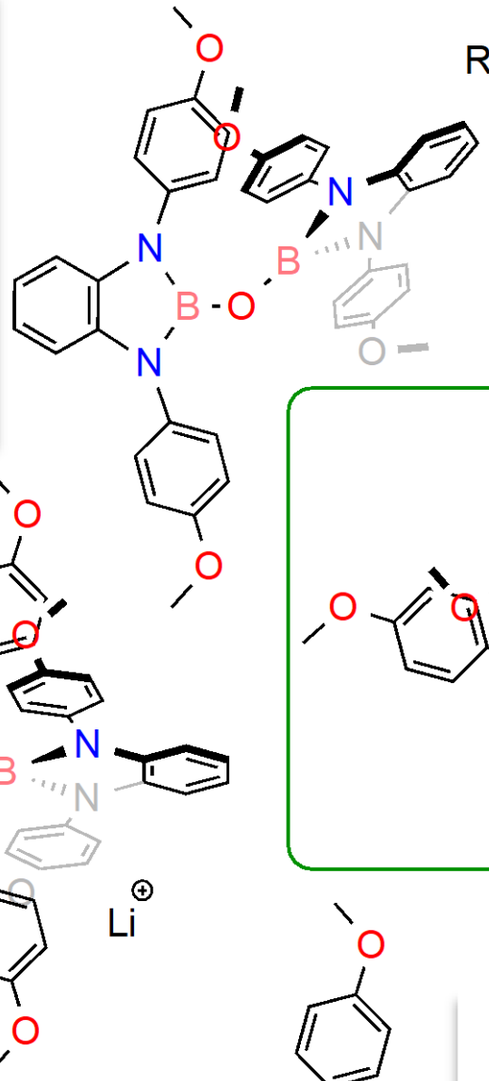
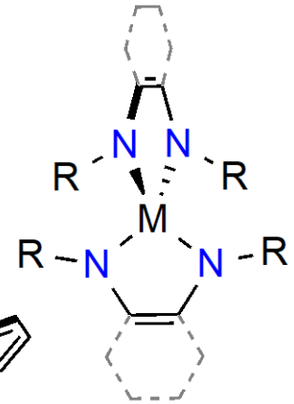
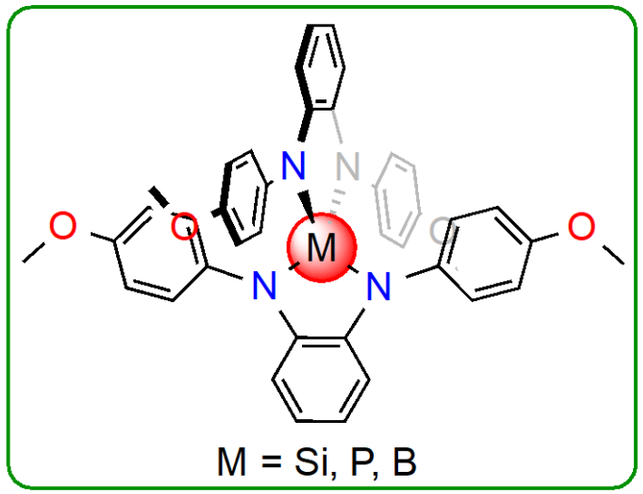
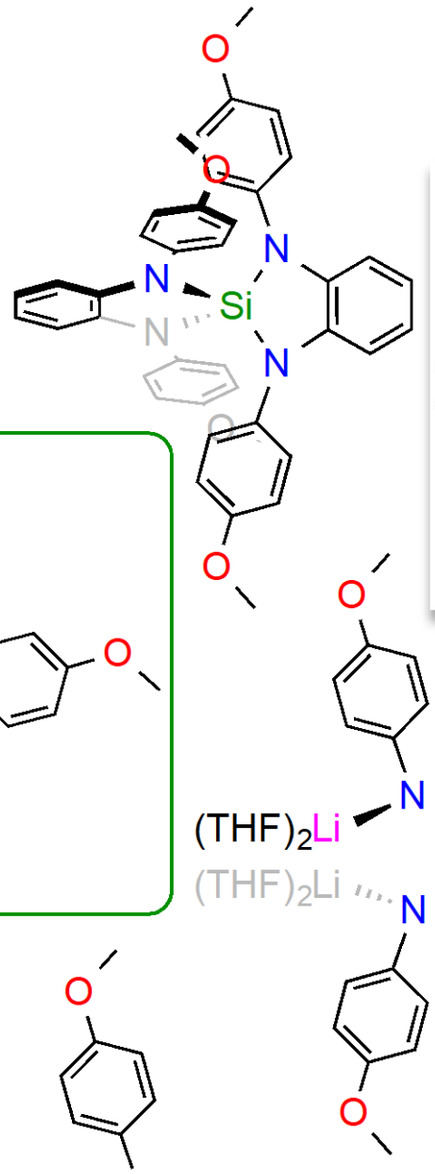
Candidates and Progress

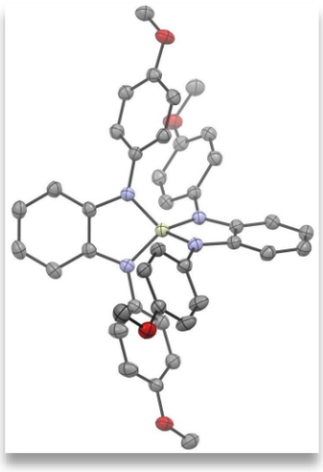


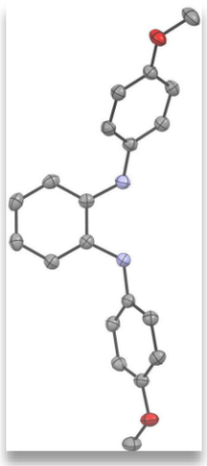


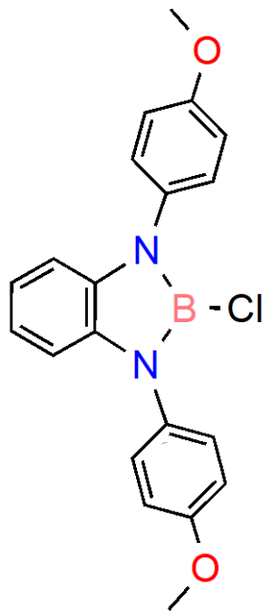


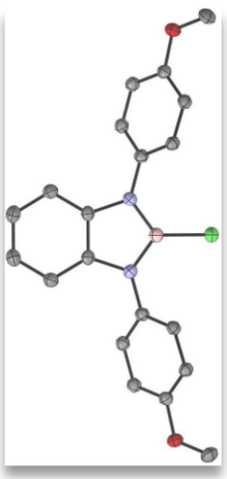


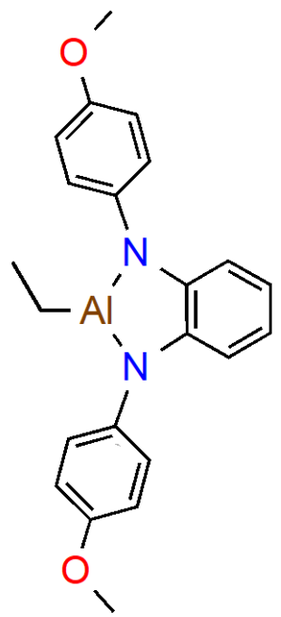


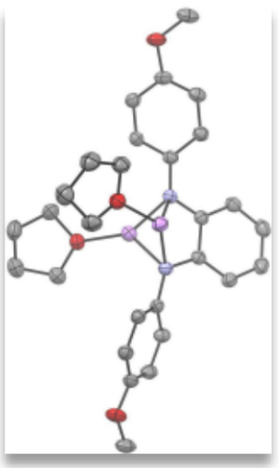












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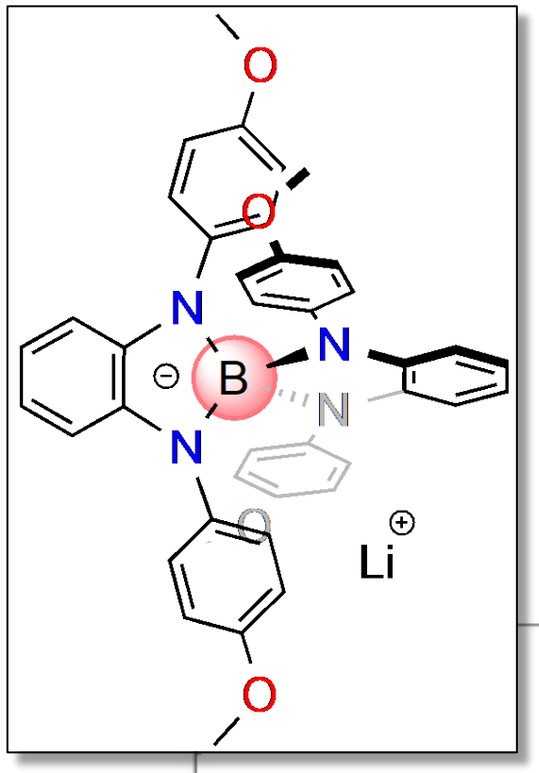
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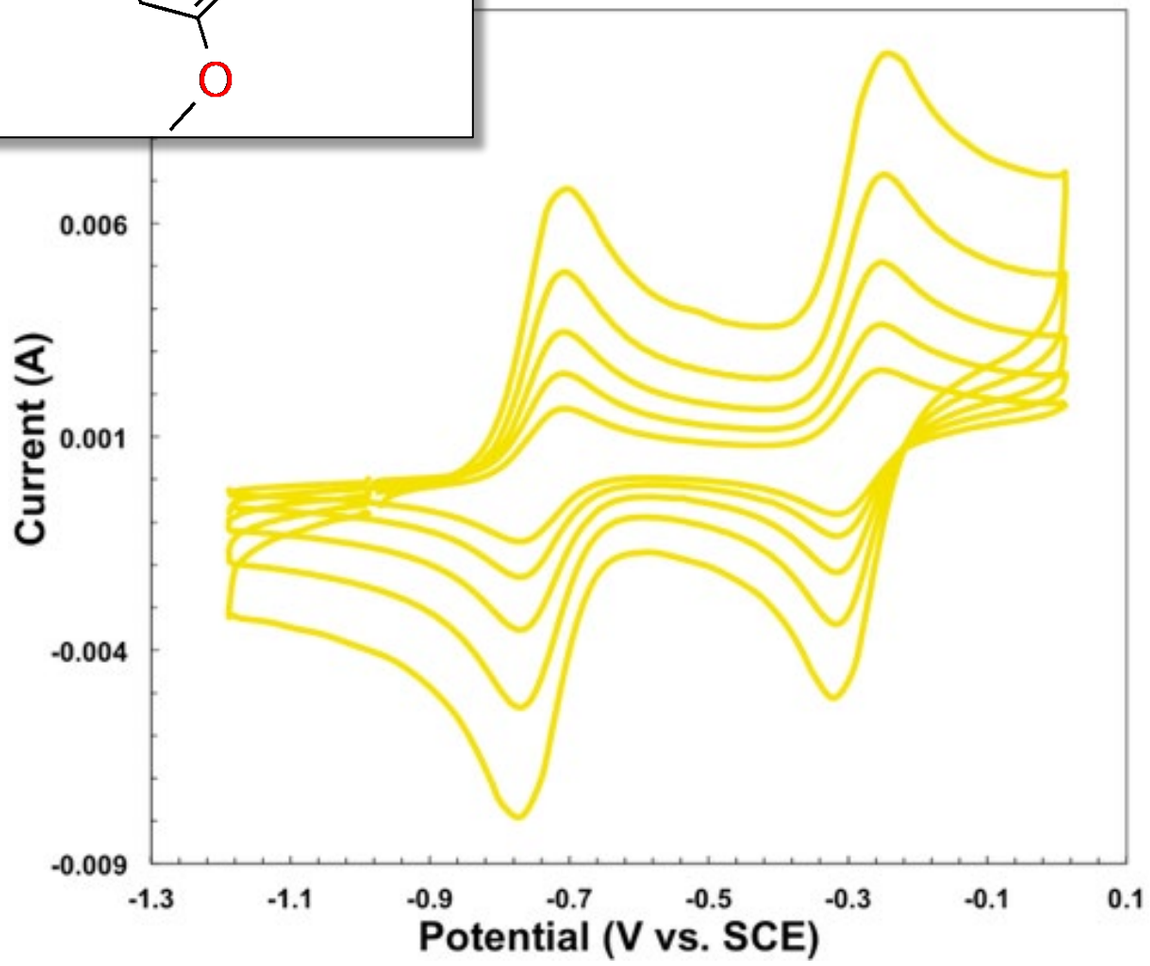
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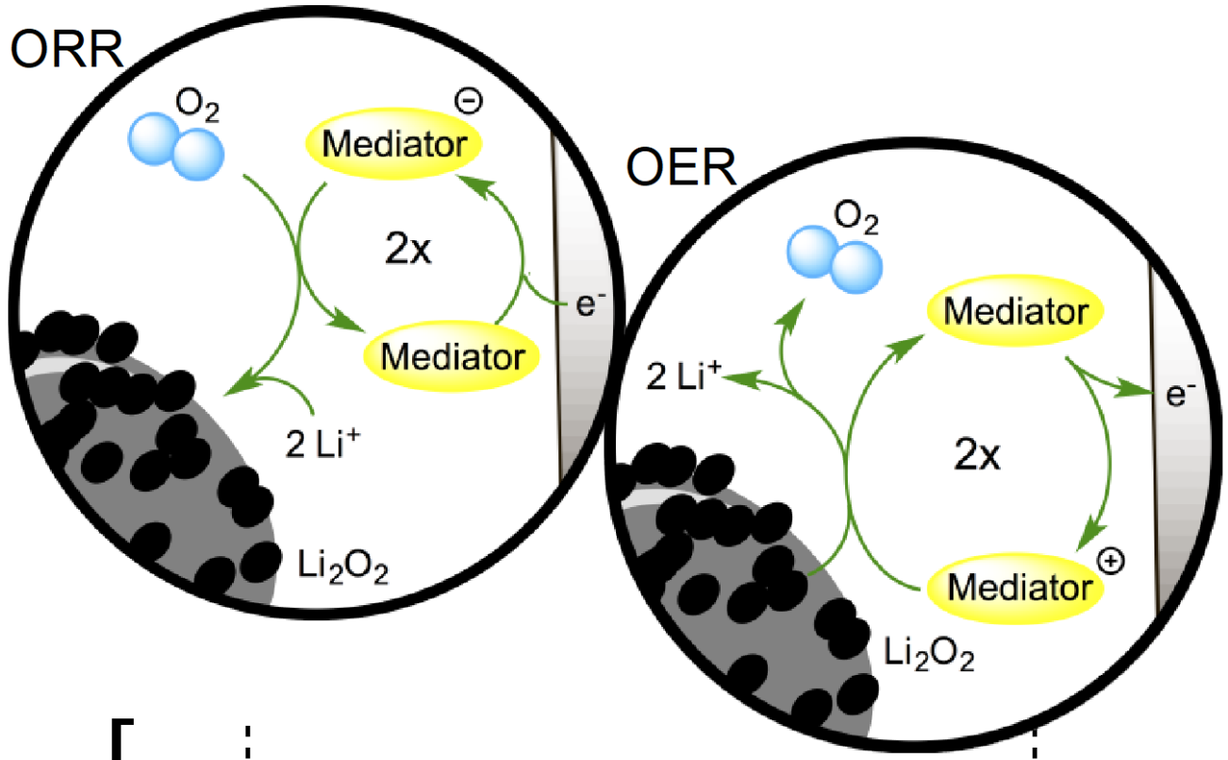
Potential (V vs. SCE)


ORR
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Mediator
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O2
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Mediator
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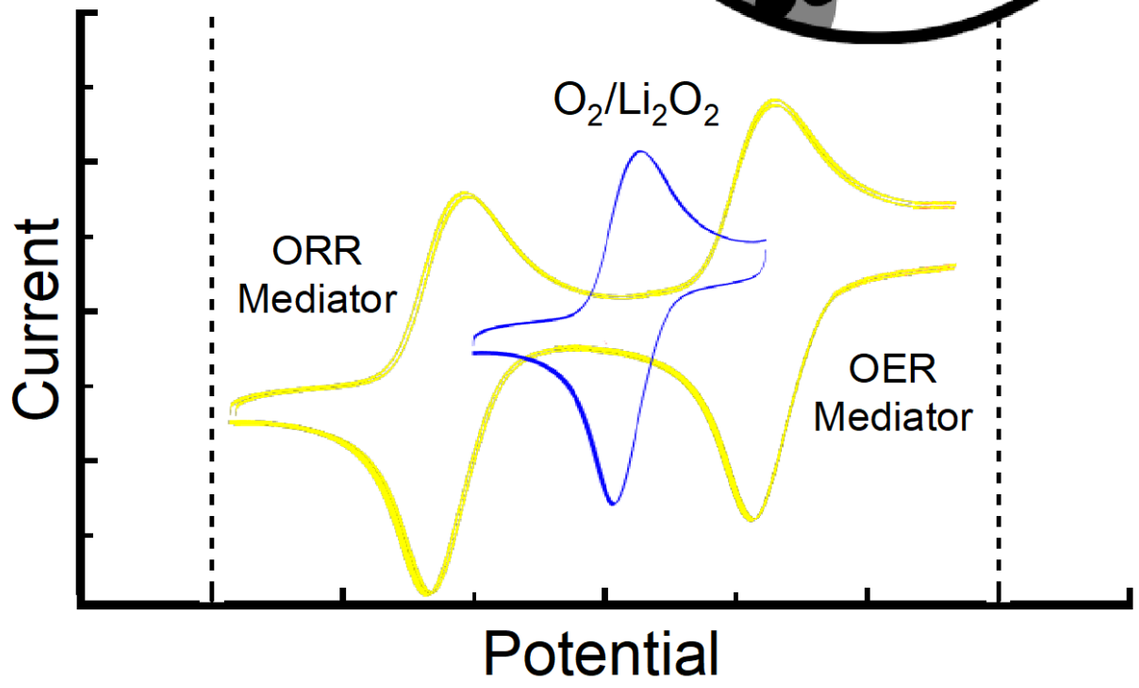
O2/Li2O2
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Potential

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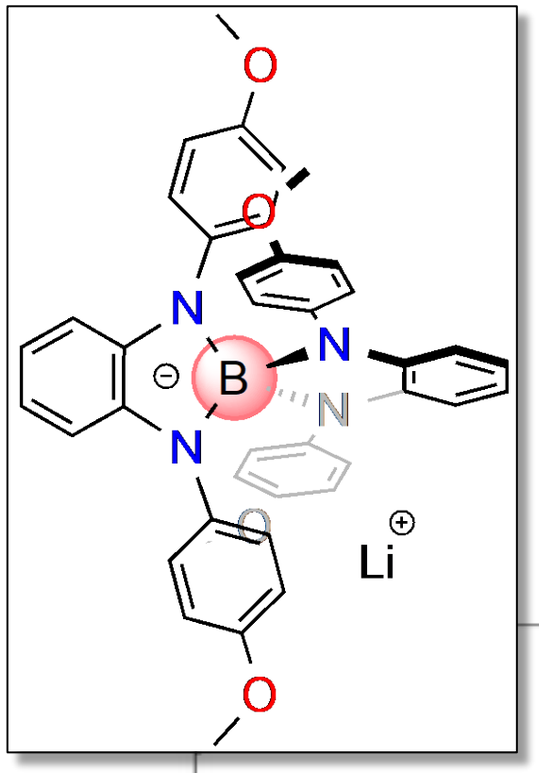
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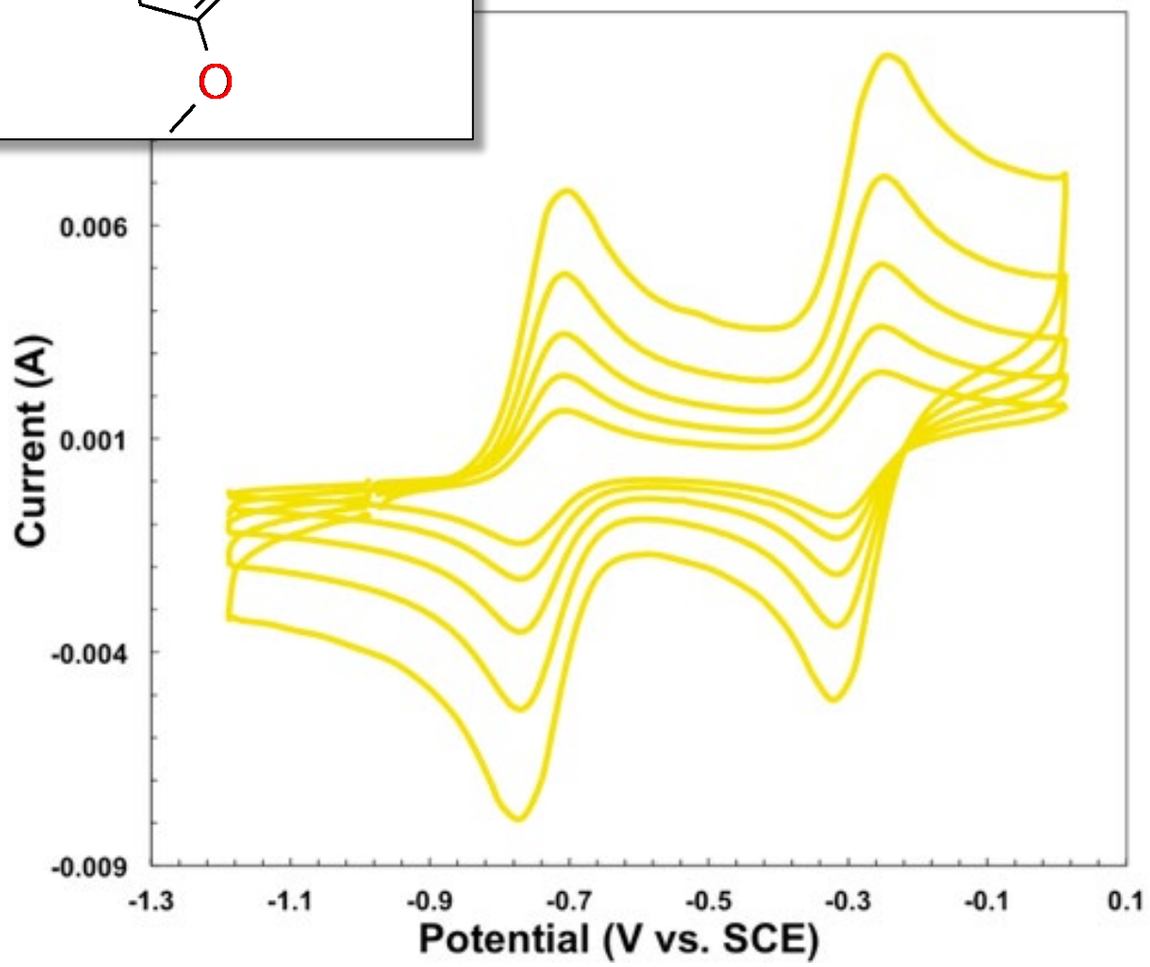
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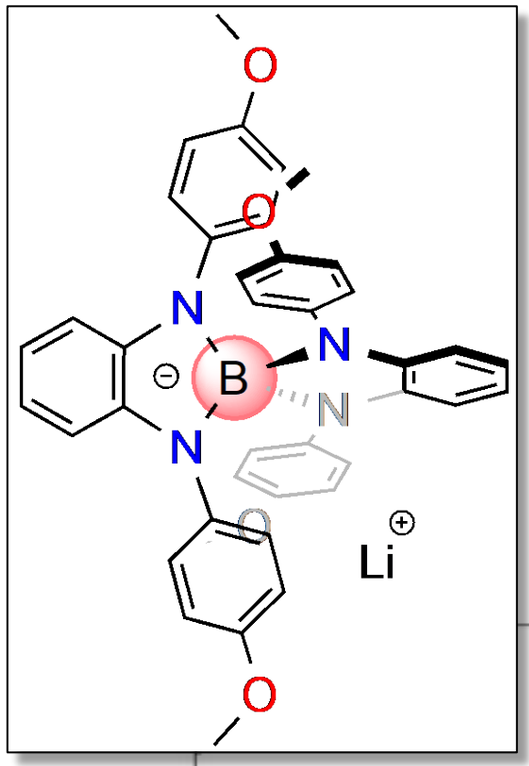
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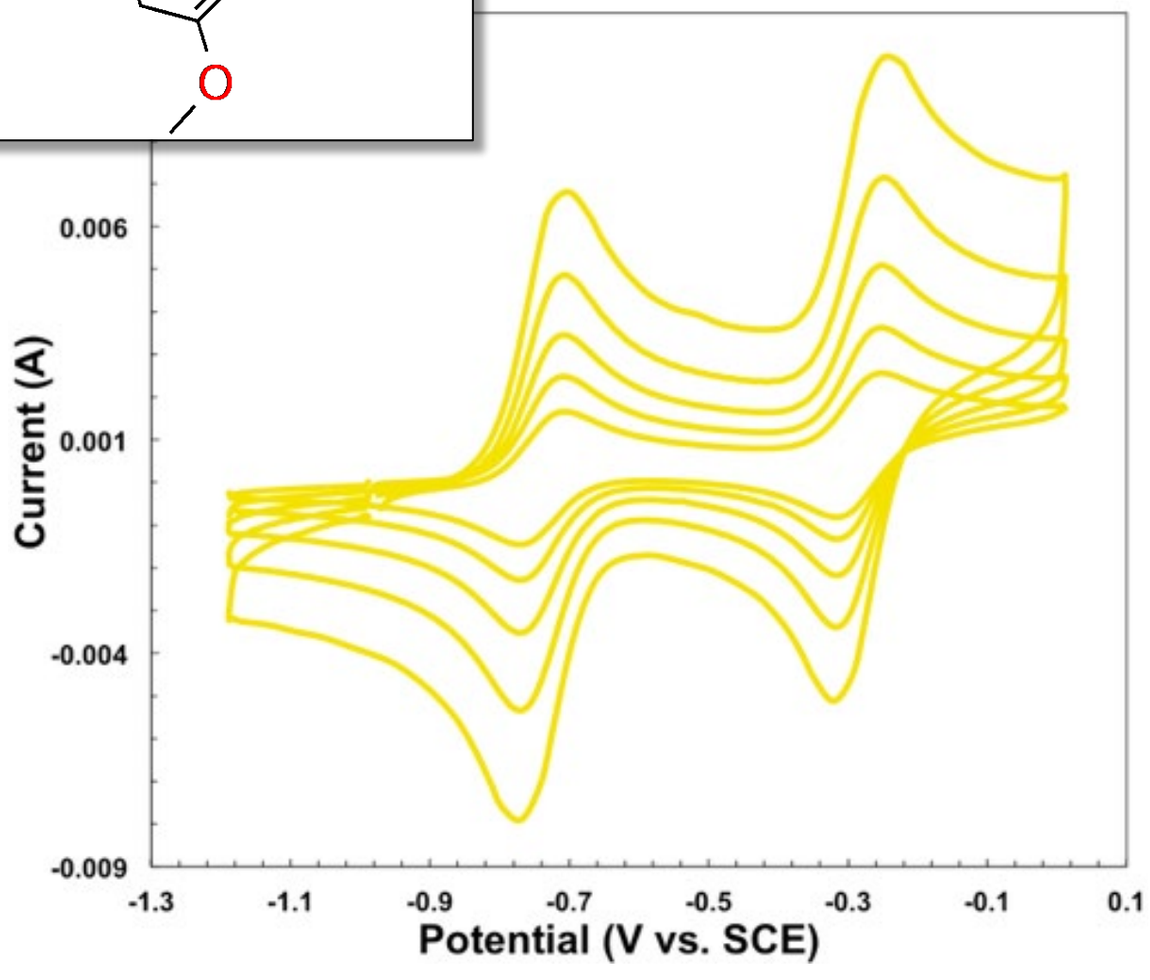
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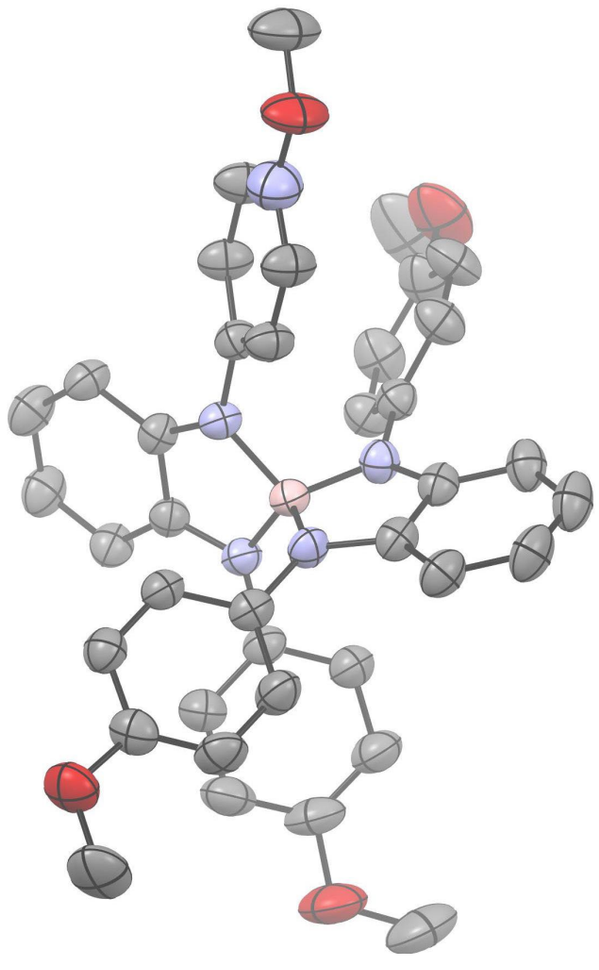

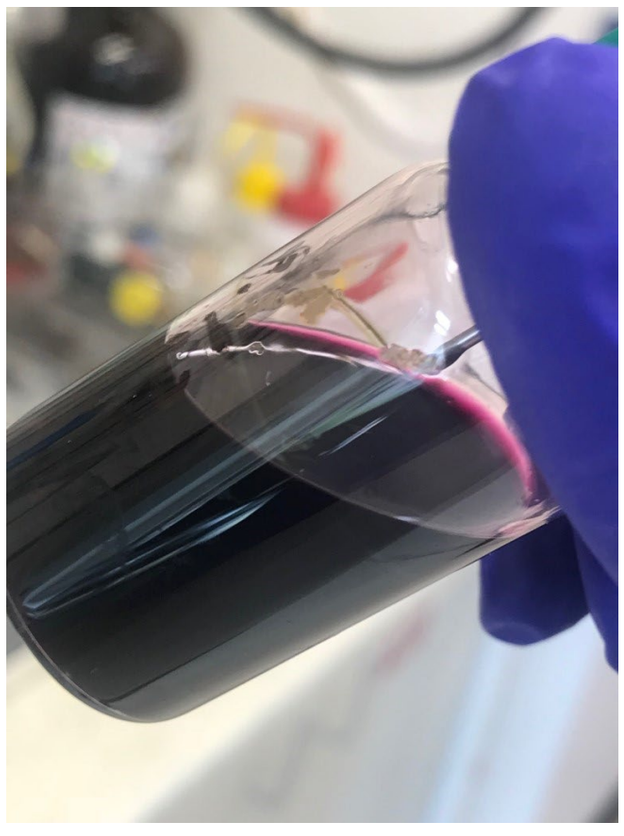

Thank you!

Questions?