Electrochemical Energy Storage through Ligand-Based Charge Manipulation

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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

Current Applications and Projects:
• New Electrolyte Development for RFB
• Redox Shuttles for Overcharge Protection
• Redox Shuttles to Enhance Charge Mobility
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Undergraduate Researchers
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Lucas Kane ('18)
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Jennie Goodell ('19)
Nick Kennedy ('19)
Claudia Hernandez ('20)
David Thole ('21)
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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
Electrolyte Design
Electrolyte Design
Based on molecular modeling, this is the charge center of the ligand.
Electrolyte Design

Two charge centers…

…displaced from one another by a “large” distance.
Target Compound
Full procedure:
31% yield, 5 grams

Performed by undergraduate students

Claudia Hernandez ('20)
David Thole ('21)
Next Steps

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)
Lucas Kane (‘18)
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Electrochemically generated radical cation in DCM
Redox Shuttles for Overcharge Protection

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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
Direct Hit!
Direct Hit!
Direct Hit!
Thank you!

Questions?