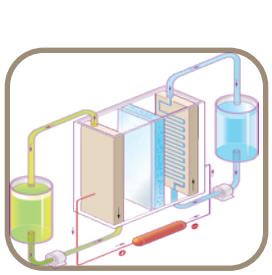

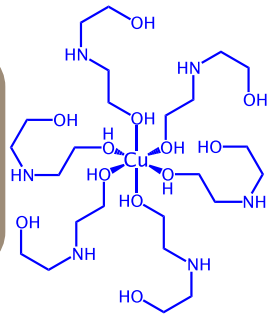

Advanced Materials for Flow Batteries

Friday, September 28, 2012

Travis M. Anderson and Harry D. Pratt III

Sandia National Laboratories

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NNSA National Nuclear Security Administration

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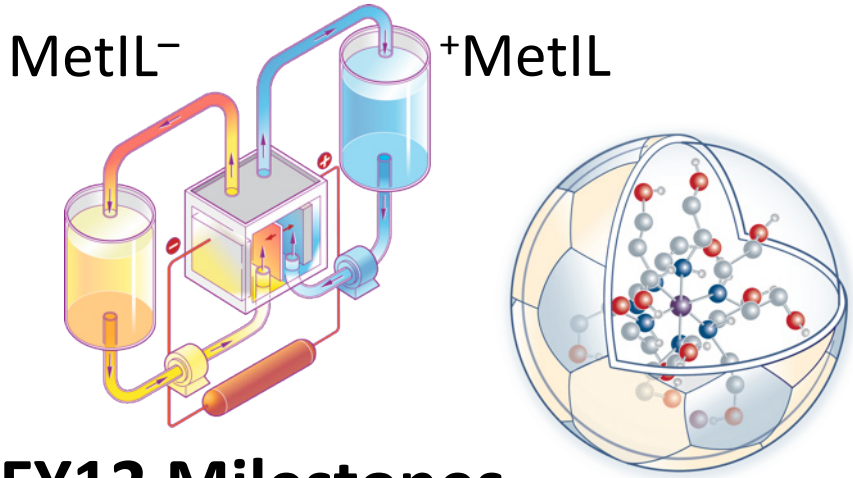
Ionic Liquid Flow Batteries

Problem: Getting high concentrations of redox active species.

Approach: Design electrolytes with charge storage species as part of their chemical composition.

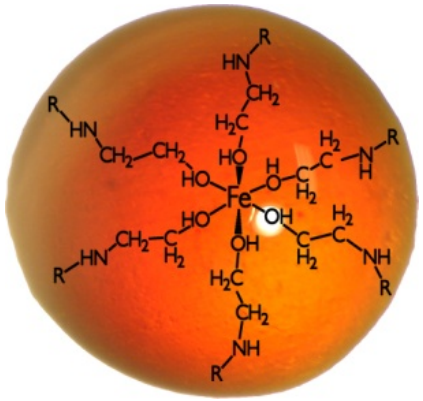


FY12 Milestones

- **59 mV/n separation (ideally n > 1)**
- **Viscosity < 500 cP**
- **Conductivity > 0.5 mS cm^{-1}**
- **Open Circuit Potential > 1.5 V**

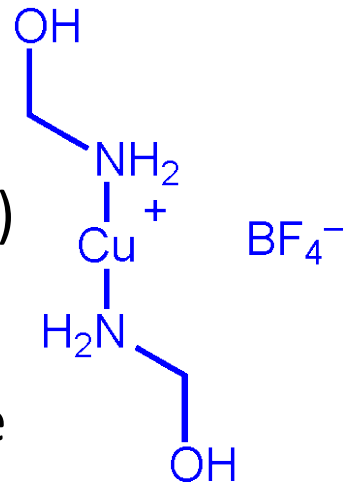
MetILs

- Transition Metal Cation
- Weakly Coordinating Anions
- Alkanolamine Ligands
- Negligible Vapor Pressure
- Non-toxic



Energy Density/Costs

SNL APPROACH: Consider a compound CuL_2BF_4 (L = methanolamine, MW = 47 g/mol), measured density 1.6 g/mL, formula weight, 244 g/mol

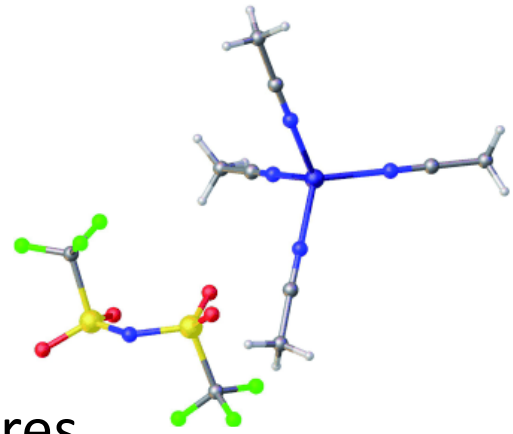


What is the molarity of redox active metal?

Divide density by formula weight (x1000 unit conversion)

6.6 M redox active copper

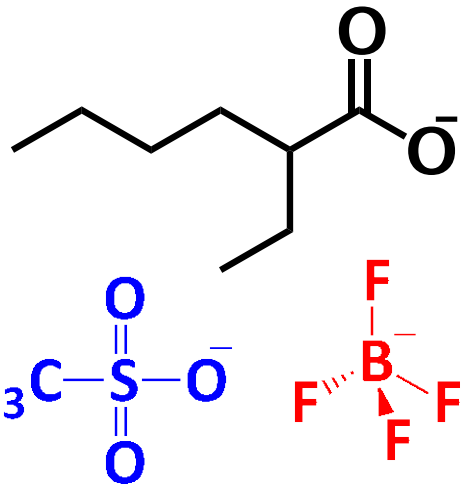
Leuven APPROACH: Prepared two- and four- coordinate MetILs with **4.5** and **3.1 M redox active copper**.



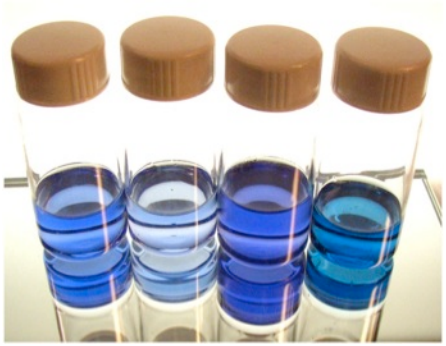
Costs:

- Higher metal concentrations/energy density
- Single-step synthesis with low cost precursors
- Higher viscosity and pump consumption can be partially offset by operating at higher temperatures.

Role of the Anion

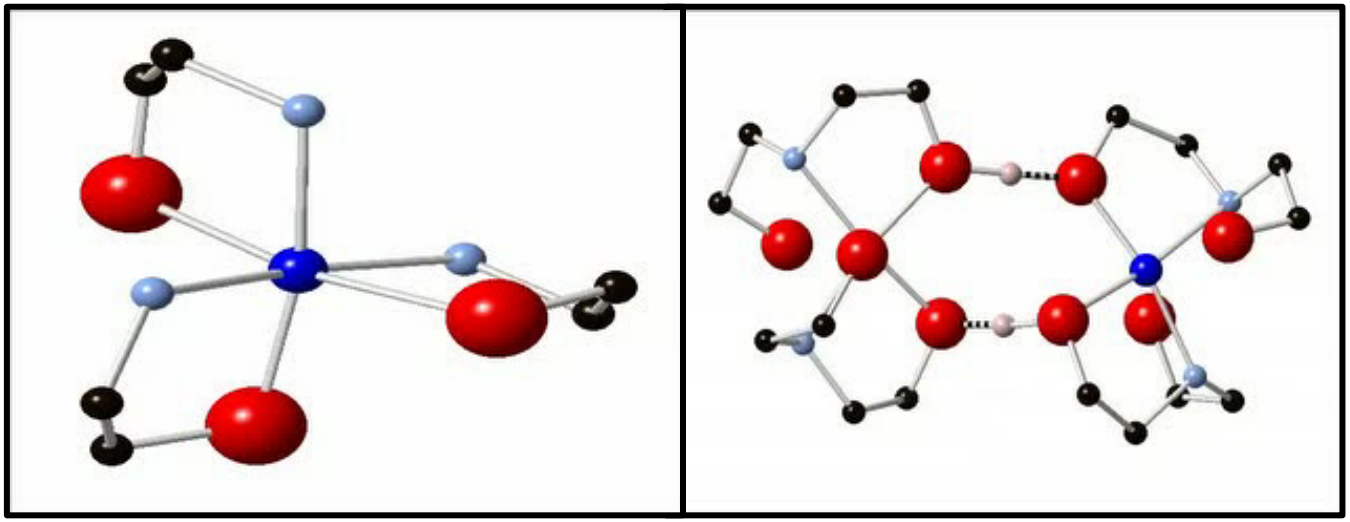


EA ethanolamine
DEA diethanolamine



Ligand	Anion 1	Anion 2	State at 25 °C	σ [mS/cm]	ΔE [mV]
EA			Liquid	0.207	244
EA			Solid	---	158
EA			Solid	---	158
EA			Liquid	6.80	102
EA			Solid	---	256
EA			Liquid	0.586	187
DEA			Liquid	0.014	522
DEA			Liquid	0.067	566
DEA			Solid	---	507
DEA			Liquid	1.05	150
DEA			Liquid	0.210	159
DEA			Liquid	0.142	201

Crystal Structures

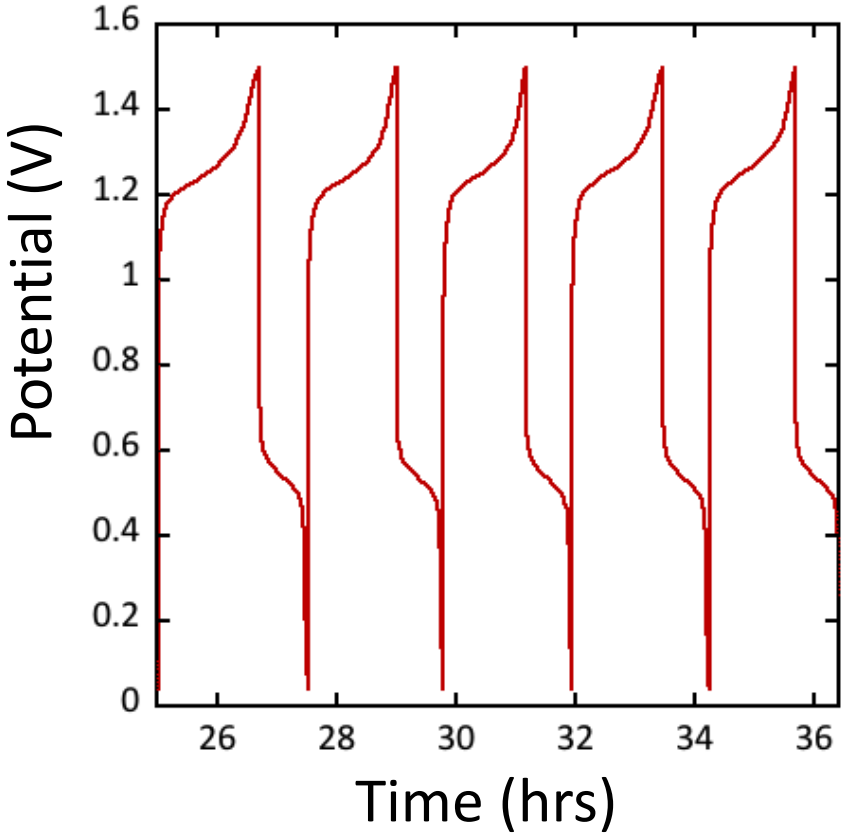


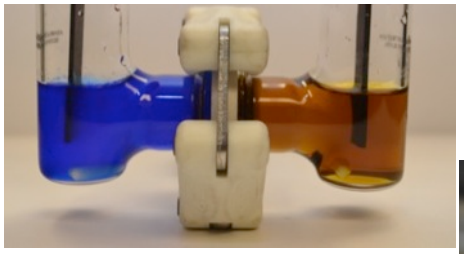
Key Accomplishments:

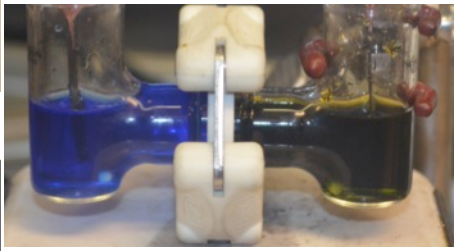
- Copper is *divalent*, complex is *monovalent*
- Alkanolamines display *non-innocence*
- Compounds still display *low melting temperatures*
- *Triflate* facilitates crystallization

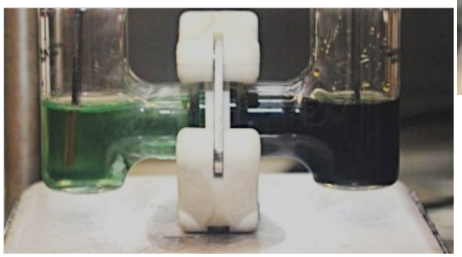
Ionic Liquid H-Cell Testing

Fe MetIL cathode
Cu MetIL anode
0.1 mA charge/discharge



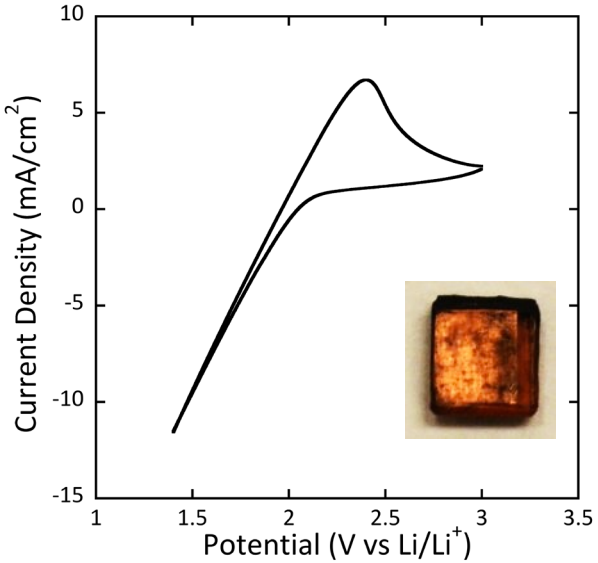


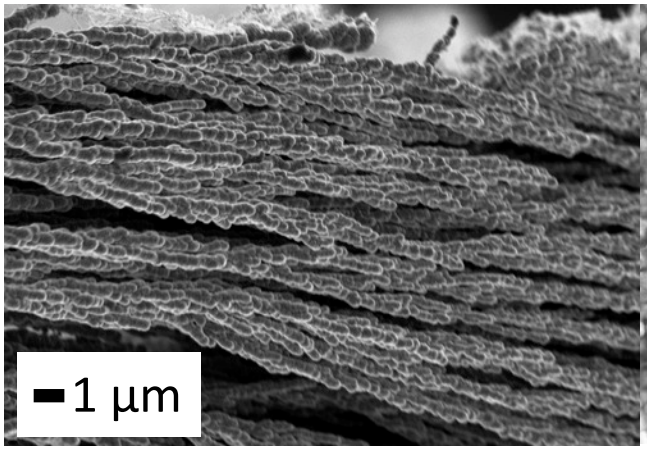




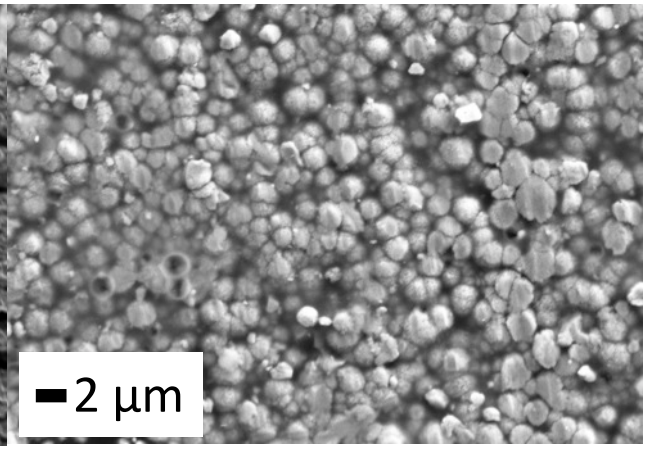
- System was validated using a literature standard.
- First tested system (Mn/Cu MetIL) resulting in reduced capacity due to copper plating.
- Improved results of a Cu MetIL/Fe MetIL system with a porous separator.

Electrodeposition

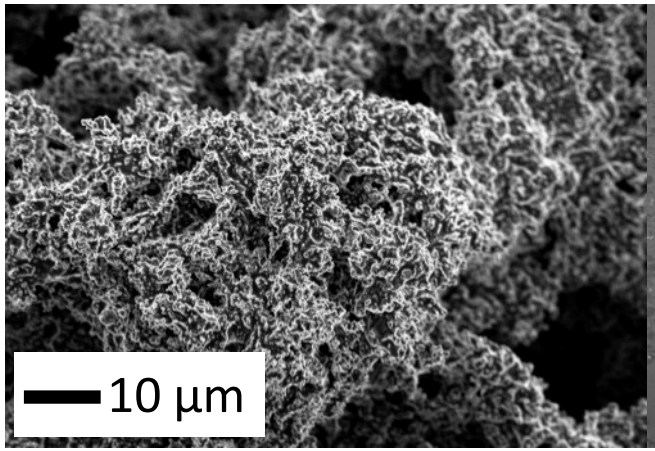




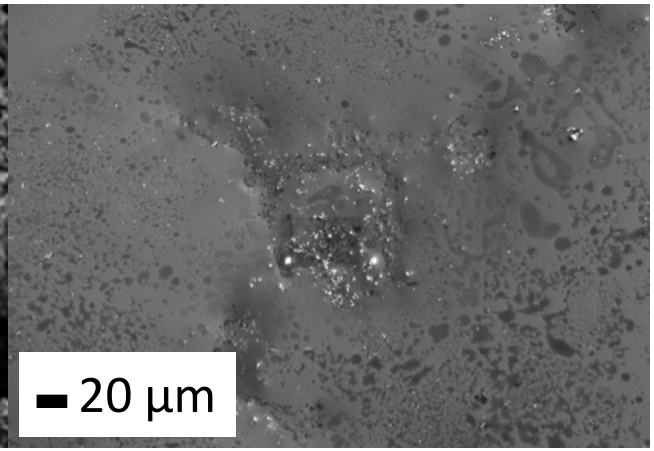
Cu—**EA**



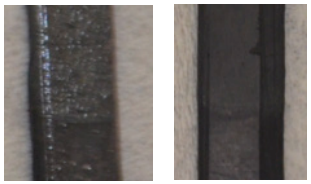
Cu—**DEA**



Zn—**EA**

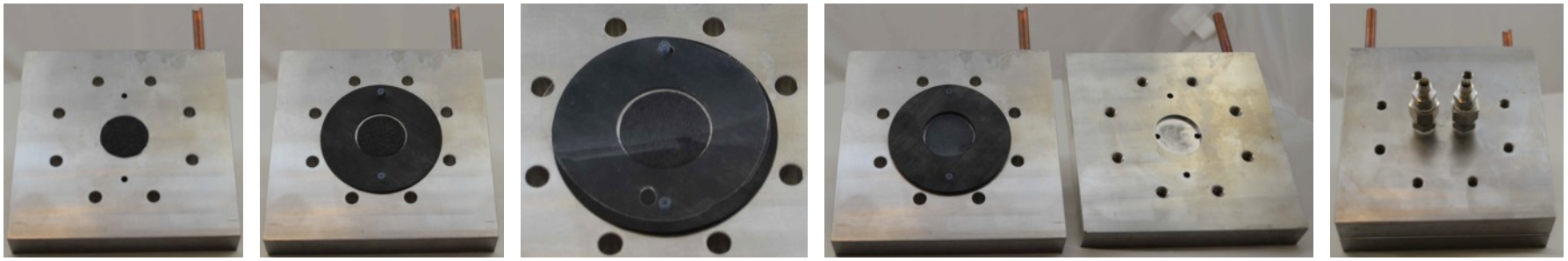


Zn—**DEA**

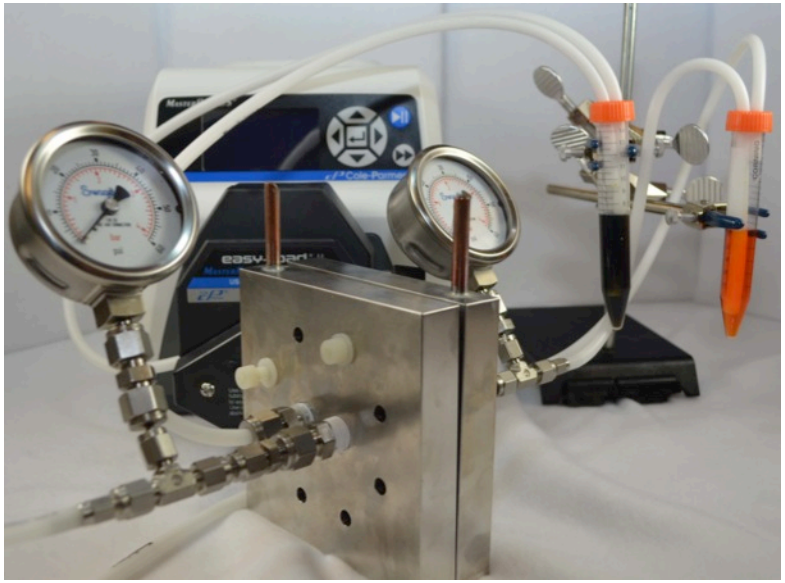


Zinc dendrite suppression with tridentate ligand

Flow Cell Tester



assembly



Key Issues:

- Force fluid against gravity
- Avoid sharp turns
- Carbon felt/membrane contact
- Wettability
- Membrane

Summary/Future Work

Sandia National Laboratories

What have we accomplished in FY12?

- Construction of flow cell testers designed to accommodate ILs.
- Met milestone of establishing a cell with high electrochemical reversibility, viscosity under 500 cP, conductivity greater than 0.5 mS cm^{-1}, and open circuit potential of 1.6 V.
- Enhanced spectroscopic tools for improved structure determination and controlling chemical properties.
- Filed a patent.

What are our plans for FY13?

- Continued testing of our suite of MetILs to identify the best candidates.
- Development of new MetILs with non-innocent ligand technology.
- Electrode and separator research to improve compatibility with ionic liquids.

Acknowledgements

Dr. Imre Gyuk

Energy Storage Systems Program Manager
Department of Energy
Office of Electricity Delivery and Energy Reliability

Technical Team:

Jonathan Leonard, Chad Staiger, and Nick Hudak

SNL Management:

Ross Guttromson, Tony Martino, Terry Aselage, and Tom Wunsch

Sandia National Laboratories
PO Box 5800, MS0614
Albuquerque, NM 87185
tmander@sandia.gov