Hybrid Electrolytes for PHEV Applications

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NOHMs TECHNOLOGIES

Rochester, NY

DOE Technical Merit Review

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Project ID: ES290

Overview

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Timeline

- Start date: 08/15/2015
- End date: 02/14/2017
- Percent complete: 44%

Budget

- Total project funding: $1,639,044
  - DOE share: $819,522
  - NOHMs: $819,522
- FY 2015: $278,481
- FY 2016: $1,269,215 (Est)

Barriers

- Electrolyte High voltage stability: stable at 4.5 to 5V
- Electrolyte Cost : <$10/kg
- Electrolyte Safety: Non-flammable and safe
- Wide temperature performance of electrolyte: @ -30^{o}C to 60^{o}C

Collaborators

- A123 - Cell Build and Testing
- CoorsTek – Ionic liquid Synthesis and Cost Analysis

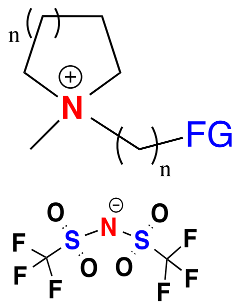
Relevance and Project Objectives

- Significant barriers to commercialization of new battery technology include:
  - Use of high voltage electrodes with stable high voltage electrolytes
  - Demonstrate low-cost manufacturability of the electrolyte at large volumes.
- NOHMs Objective is to develop functional ionic liquid based electrolytes that exhibit high conductivity, excellent electrode stability and wide temperature operations for applications in 5V Li-ion batteries
  - Functional ionic liquid design and synthesis
  - “5.0 V” Electrolyte formulation and optimization
  - Prototype cell assembly and testing (2Ah) (NMO, NMC532)
  - Design and cost study of electrolyte production
  - Building 10Ah pouch cells for USABC final deliverables (NMO, NMC532)

Milestones

Milestone	Timeline (Quarters) 1	2	3	4	5	6	Status
Synthesize ILs with high purity and formulations that are 5V stability. Characterize electrolyte formulations: viscosity < 5cP and 5 V stability in coin cells and SLP cells							On Track and On-going
Coin and Single Layer Pouch cell testing with A123. Down select electrolytes based on performance							On Track and On-going
Electrolyte formulations showing 5V stability and high temperature (@ 60 °C) stability at C/3-rate. Deliver to USABC 2 Ah pouch cells (30 cells, 2 electrolytes, 15 cells of each electrolyte)							Go/No Go decision point after results from USABC
Two Electrolyte formulations showing 5 V stability and low temp stability (@ -30 °C)							Future Work
Cost analysis and delivering cells for testing. 10 Ah pouch cells, with 2 electrolytes, 15 cells/electrolyte							Future Work

Approach/Strategy



Functional ionic liquid design/synthesis (CoorsTek, NOHMs Technologies)

Electrolyte formulation design (NOHMs Technologies)

- ✓ Statistical tools: DOE
- ✓ Literature
- ✓ NOHMs technical knowledge

Transport & Electrochemical property measurements (NOHMs Technologies)

- ✓ Viscosity, conductivity
- ✓ Floating current studies >5V
- ✓ Graphite SEI formation
- ✓ Low ICL

Coin & Small pouch cell testing (A123 Venture Technologies, NOHMs Technologies)

- ✓ Half cells, full cells
- ✓ EIS studies
- ✓ FTIR, SEM, XPS studies

Pouch cell testing

(2Ah and 10 Ah pouch cells) (A123 Venture Technologies)

Electrolyte cost estimation and manufacturing (CoorsTek, NOHMs Technologies)

Technical Accomplishment:
NOHMs Novel Ionic liquids

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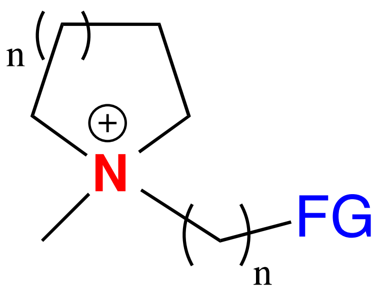
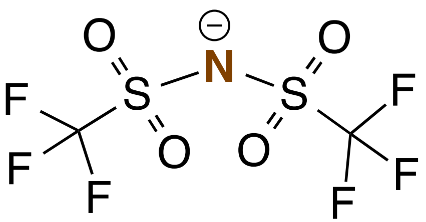
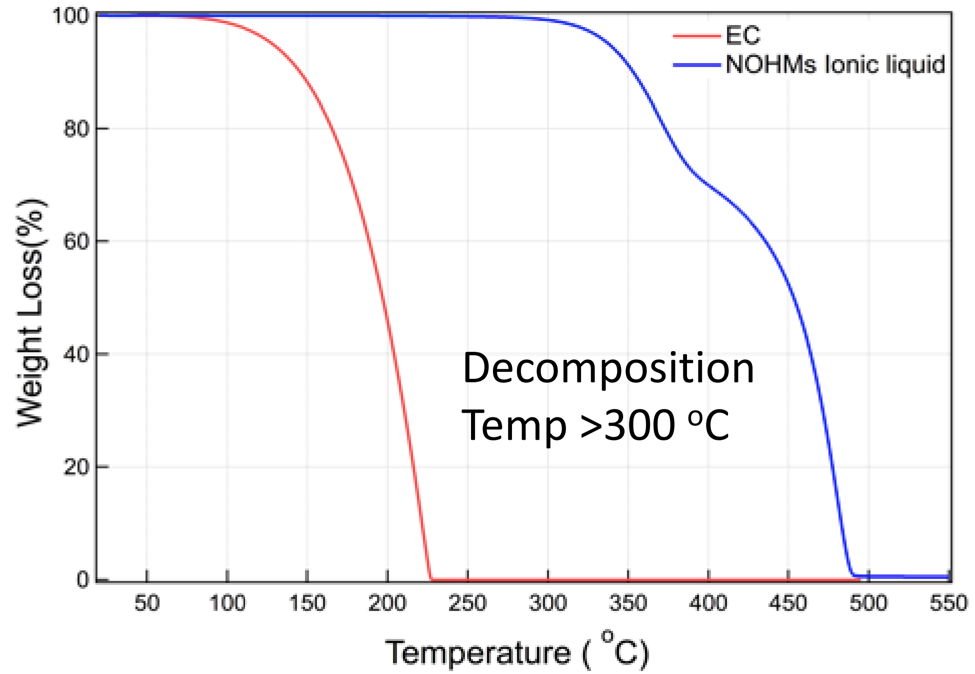


Hetro-cyclic Cation family containing a functional group

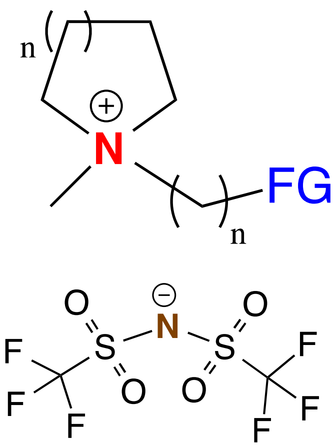


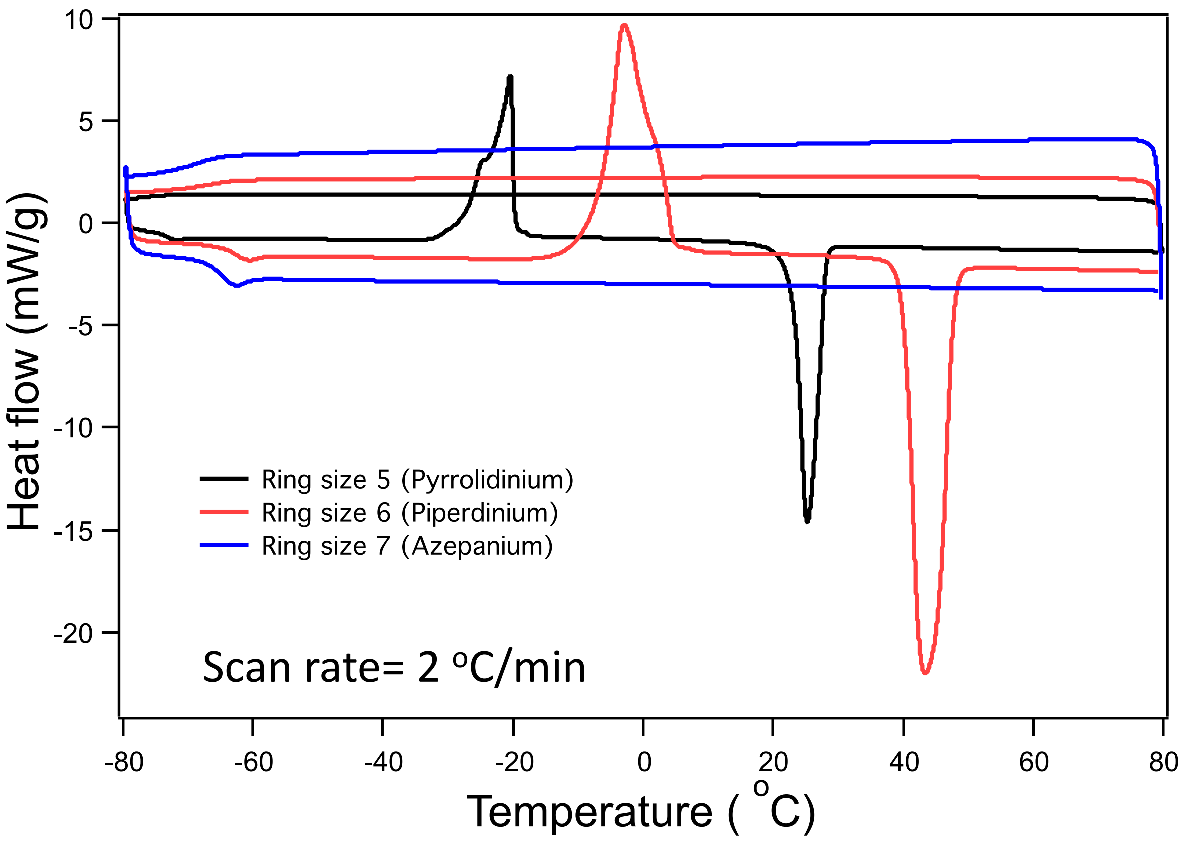
TFSI Anion



Elemental analysis (C, H, N) confirmed 99.99% purity with 0% halide concentration (ICP)

Technical Accomplishment:
NOHMs Novel Ionic liquids





Differential scanning calorimetry traces indicate larger ring size results in liquid salts with no distinctive phase transitions.

Technical Accomplishment:
Electrolyte transport properties

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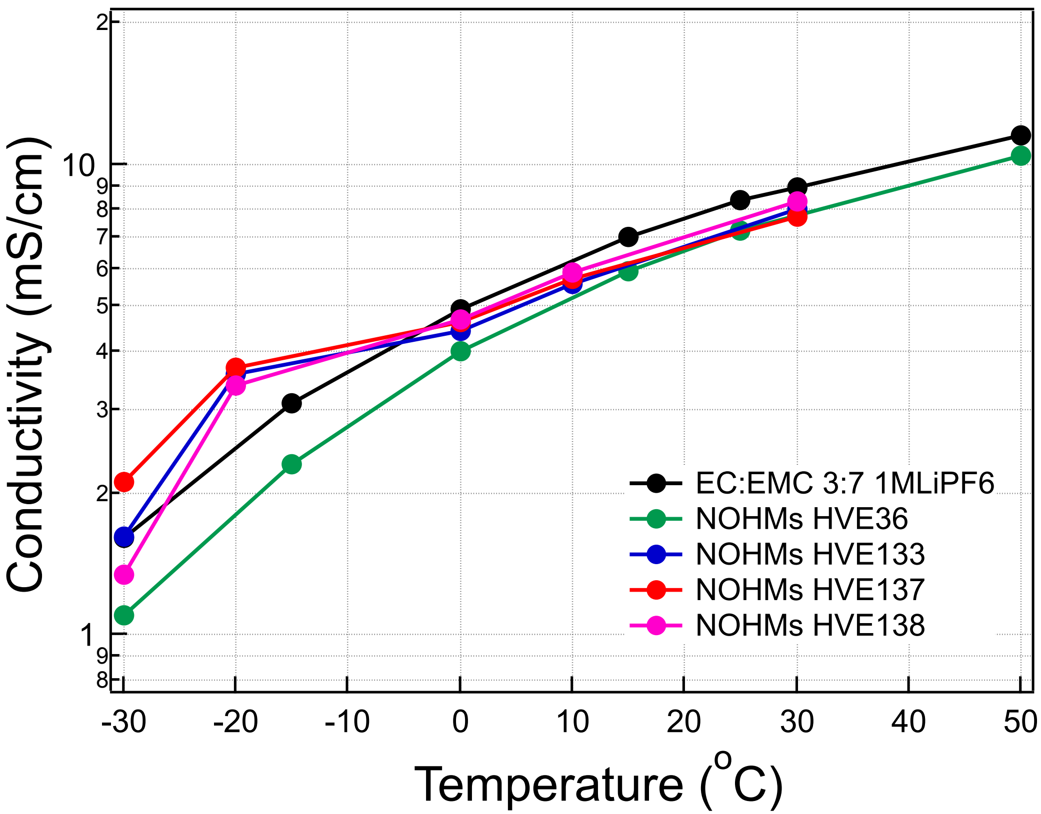
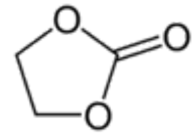
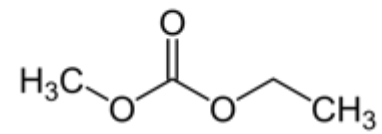
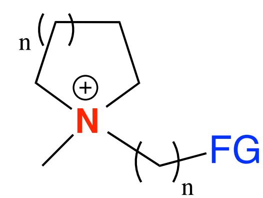




EC



EMC

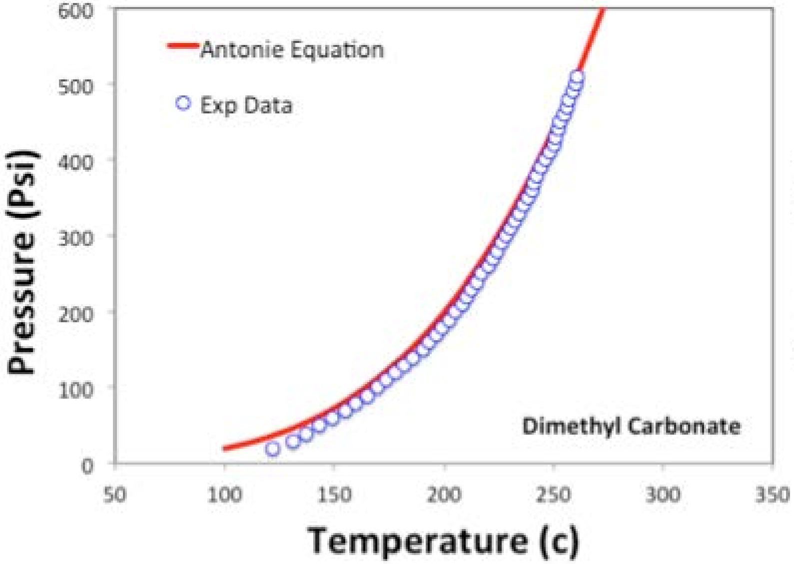


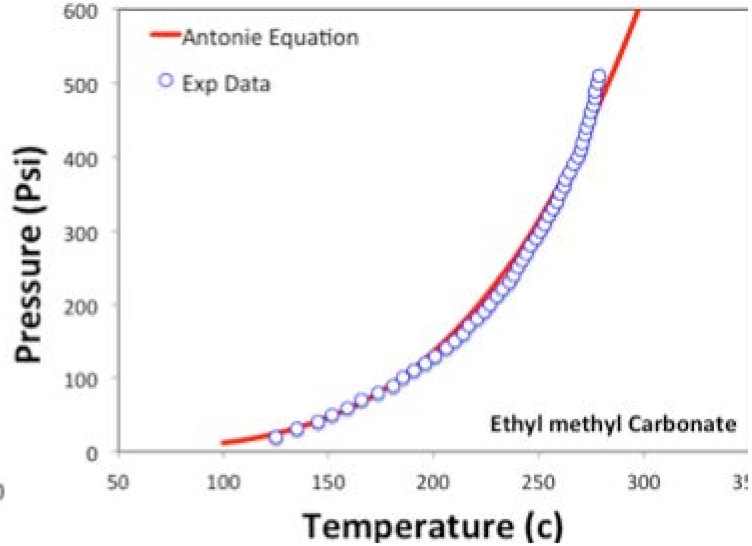
Ionic liquid

Novel functional groups to lower Ionic liquid viscosity

NOHMs Electrolyte formulation show similar conductivities compared to base line electrolyte

Technical Accomplishment:
Vapor pressure measurements

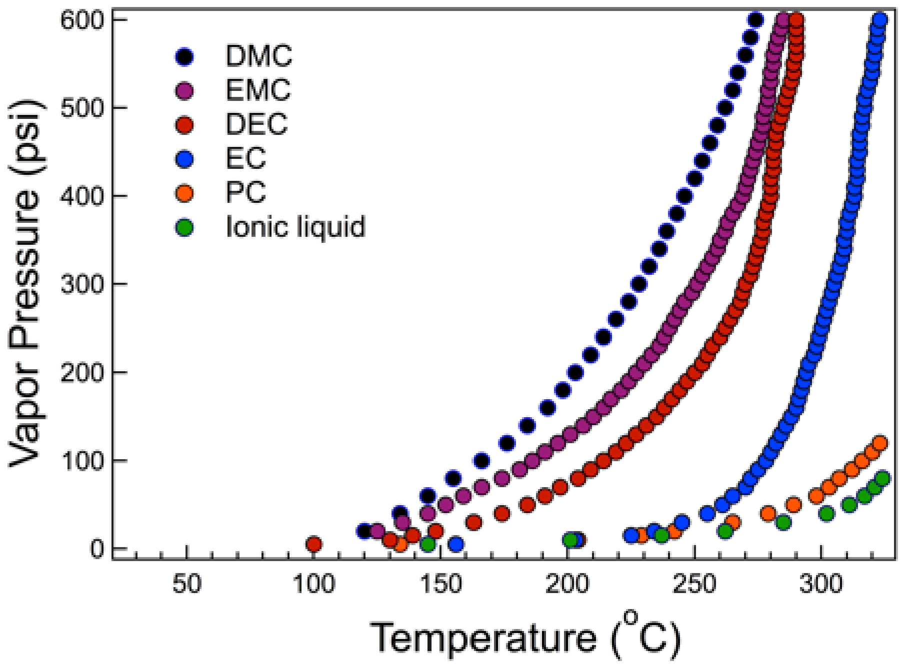


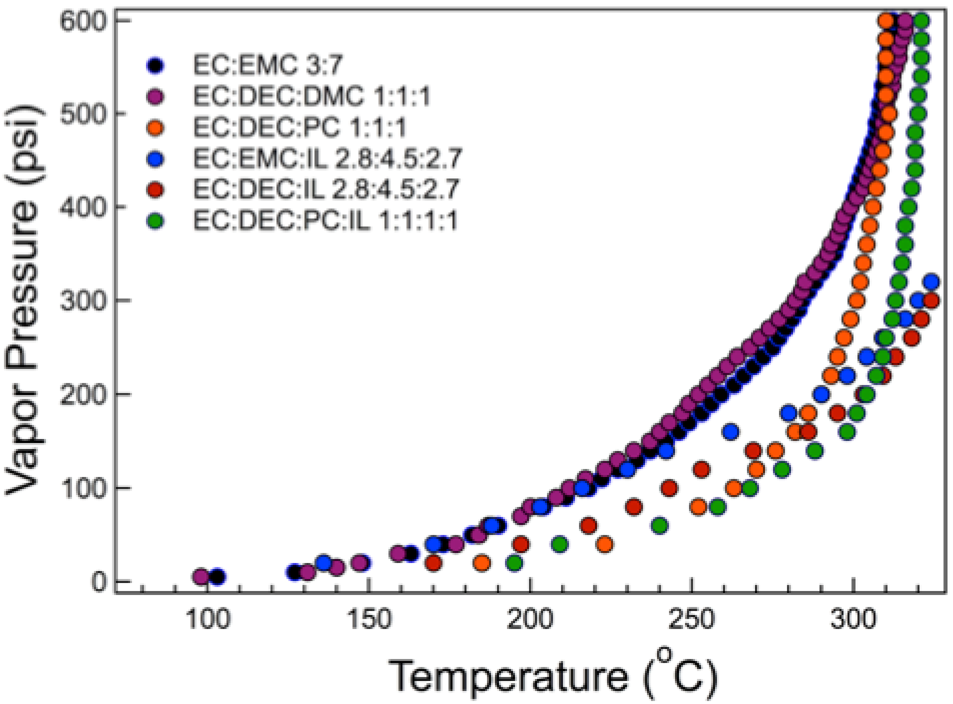


High pressure and high temperature reactor with controlled heating system is developed to collect the vapor pressure *vs* temp data

Collected experimental data matches with the Antonie equation

Technical Accomplishment:
Vapor pressure of mixtures

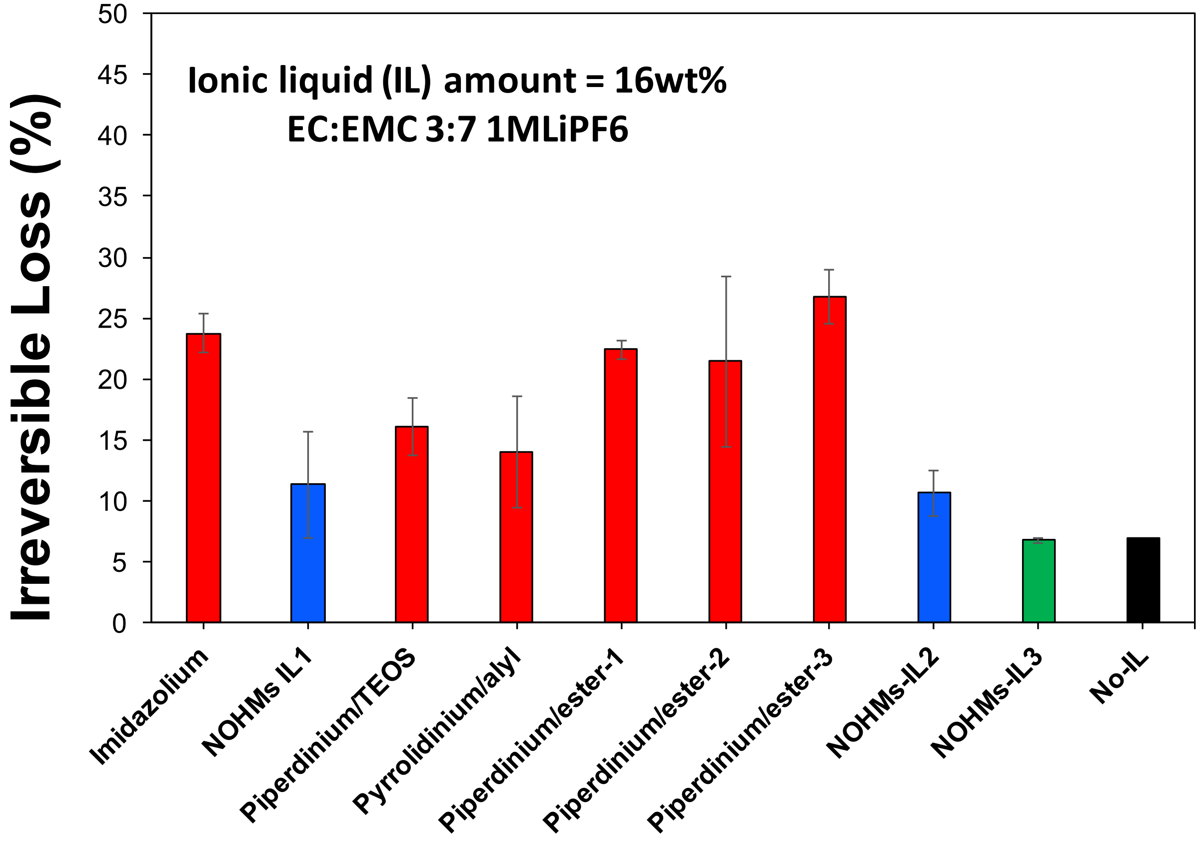




Propylene carbonate and Ionic liquid exhibited excellent thermal stability- Significantly less vapor pressure up to 300 °C

Electrolytes with PC and ionic liquid would provide considerably less volatile systems

Technical Accomplishment:
Stability against Graphite anode

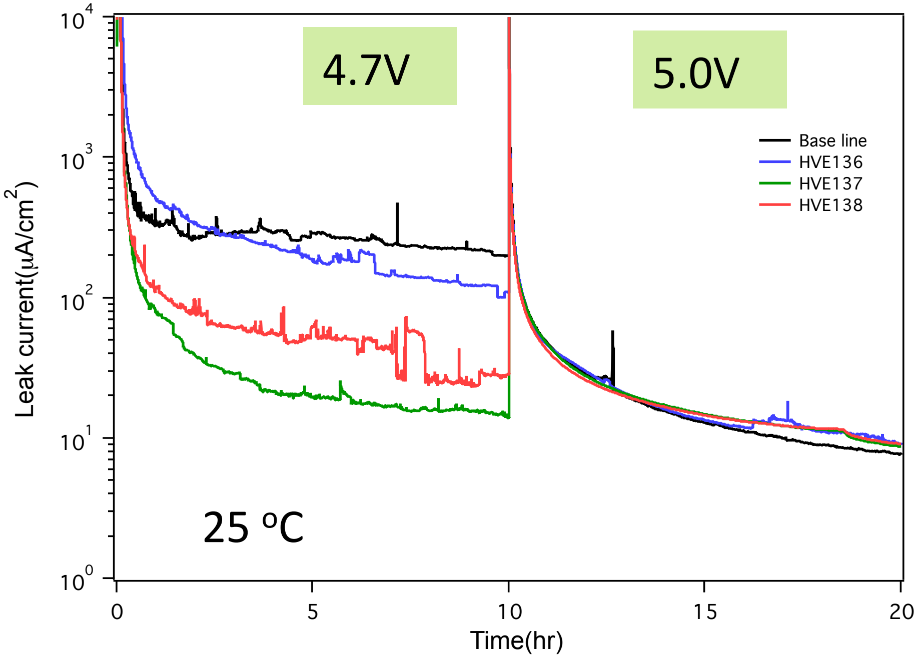


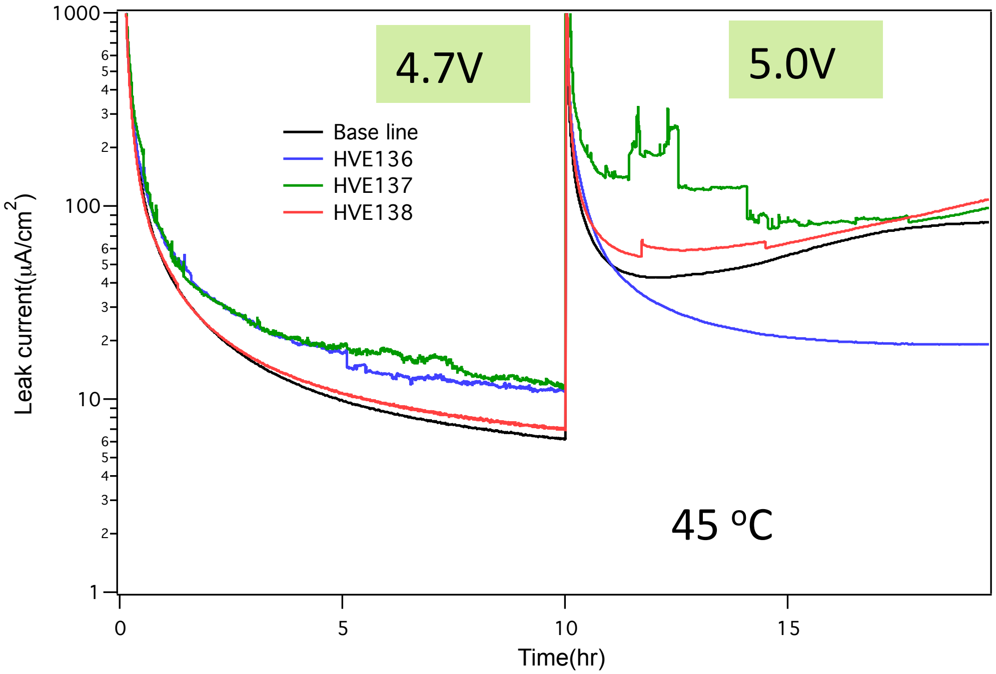
Ionic liquids are not stable against Graphite anode at low voltages

To understand the affect of IL cation type and functional group, irreversible capacity loss of Li-Graphite half cell at C/10 rate is used a screening methodology

NOHMs functional ionic liquids showed excellent reduction stability against graphite anode even at very high concentrations (16 % by mass in the electrolyte)

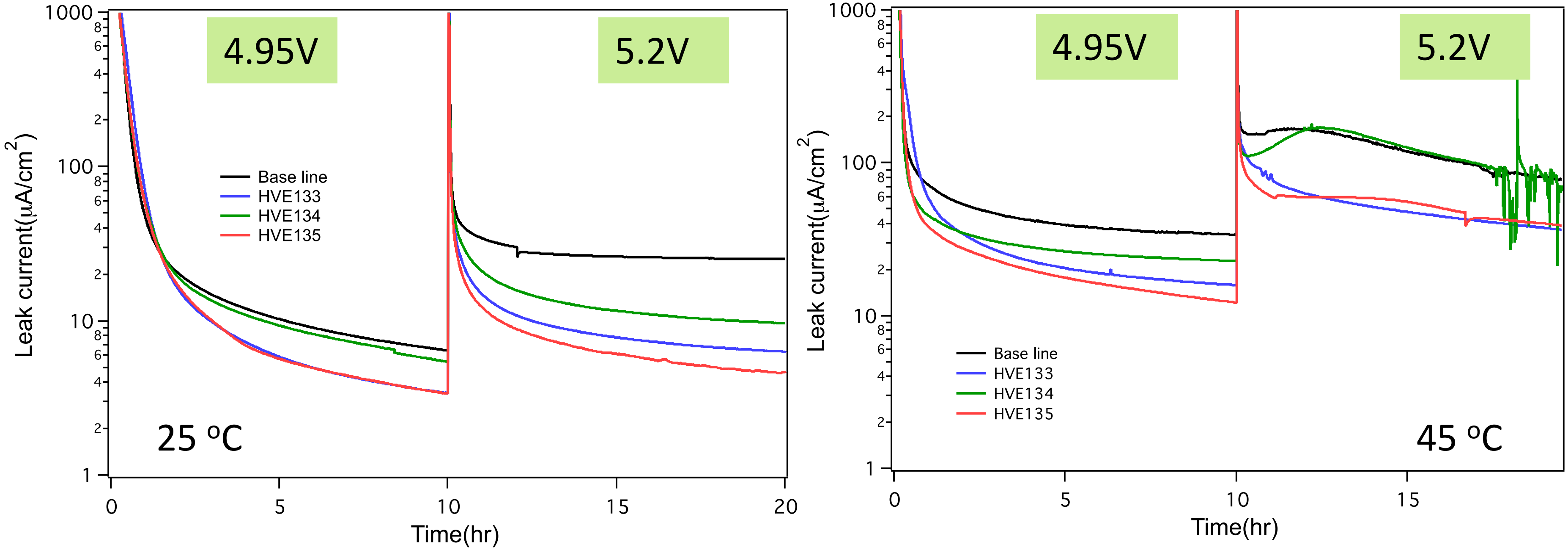
Technical Accomplishment:
Stability against NMC532





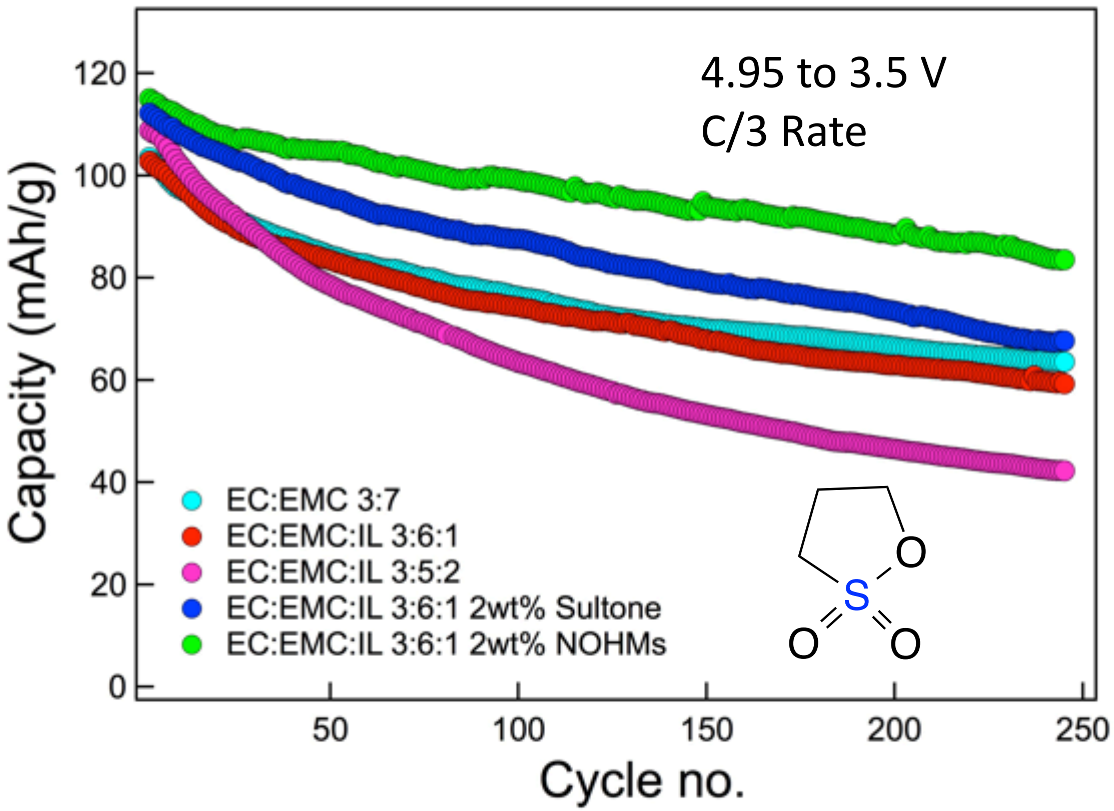
✓ NOHMs proprietary IL electrolytes showed very low leak current against NMC532 cathode even at elevated temperatures

Technical Accomplishment:
Stability against NMO



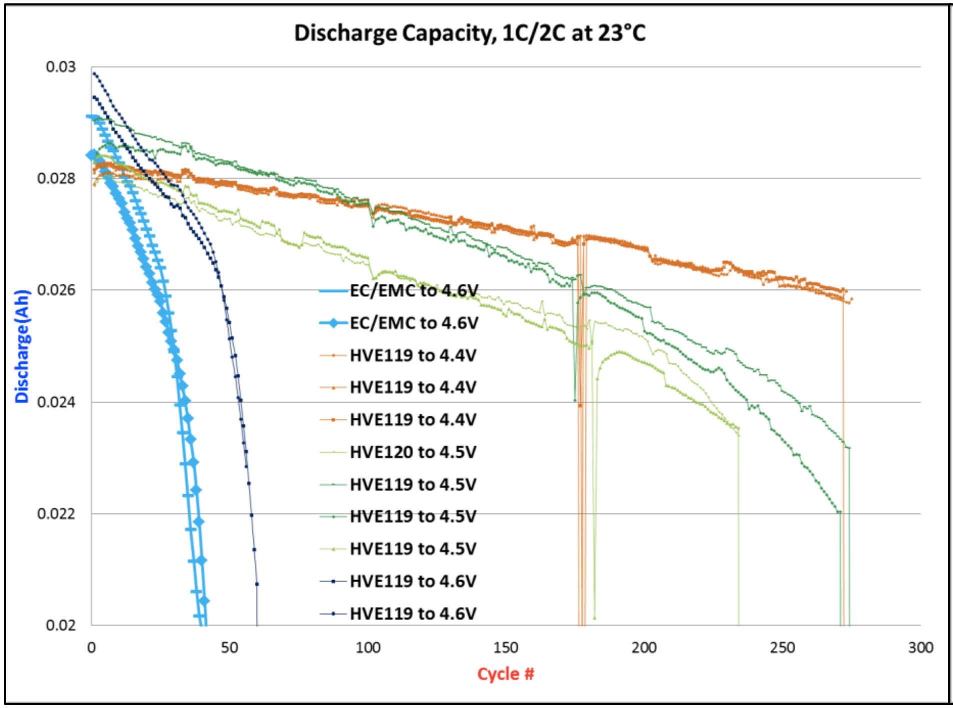
✓ NOHMs proprietary IL electrolytes showed very low leak current against NMO cathode even at elevated temperatures

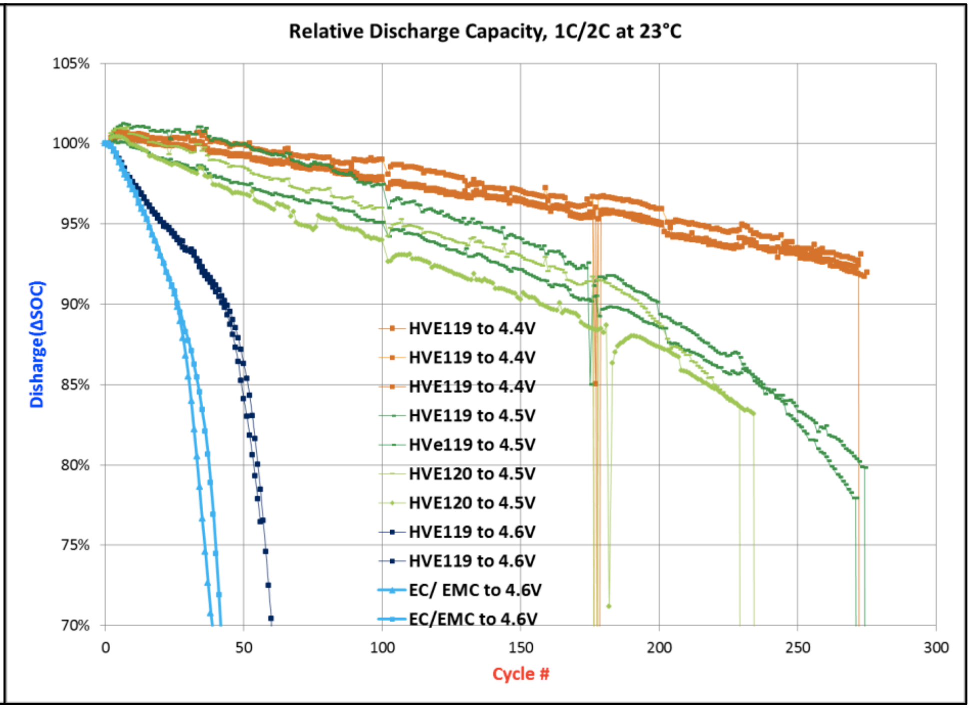
Technical Accomplishment:
NMO-Graphite- Cycling



- ✓ Base line electrolytes EC:EMC 3:7 and EC:EMC:IL 3:6:1 showed similar cycle capacity retention
- ✓ Further addition of ionic liquid lowered the capacity retention
- ✓ Additive in conjunction with NOHMs functional ionic liquid exhibited improved performance

Technical Accomplishment:
NMC532-Graphite- Voltage sensitivity





NOHMs designed electrolytes showed promise in NMC532-Graphite pouch cells at 2C discharge rate

Response to Previous Reviewers

- This is a new project and was not reviewed last year

Collaborations

- Electrode construction (NMC and NMO) and mall format cells for proof of concept
- Deliver 2 Ah and 10Ah prismatic pouch cells (NMC & NMO) with NOHMs electrolyte

- Produce small quantities of ionic liquids
- Cost Analysis of high volume electrolyte production
- New Partner TBD

Challenges and Barriers

- NMO cathode presents challenges to create high loading for 2Ah and 10 Ah cell builds
- Ionic liquid stable against cathode are not stable against graphite anode
- Additive that form a stable SEI on graphite react with NMO/NMC532 cathodes at high voltages
- Optimization of additive and functional ionic liquid combination is important to achieve high voltage stability and full cell operation

Proposed Future Work

- 2016 (Q3 & Q4)
  - Down select to the best electrolyte for NMC and NMO and make 2Ah pouch cells for USABC delivery.
  - Based on USABC test results improve on electrolyte formulation, continue Electrochemical testing and abuse tolerance testing
  - ByDec 2016 – produce liter quantities of final electrolyte for NMC and NMO
  - 2016 Q4 – Develop cost model for final electrolytes
- 2017 Q1
  - Build and Deliver sixty 10Ah pouch cells with NOHMs electrolyte (30 NMO; 30 NMC)

Summary Slide

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- Narrowed down IL based electrolytes from 130 to 10
- Promising performance Results
- Established multiple screening methods to down select electrolyte formulations

Gap Chart

Parameter		Unit	USABC Goal	NOHMs Start	NOHMs Current
Electrochemical Stability (100 µA/cm^2 threshold)	Upper Voltage	V vs. Li/Li$^+$	5	5	5.2
	Lower Voltage		0	-	0
Specific Conductivity	at 30°C	mS / cm	> 12	7	8.3
	at -30°C		> 4	1	2.0
Lithium Transference Number			> 0.35	0.25	0.36
Viscosity	at 30°C	cP	< 5	>10	<5
	at -30°C		< 20	-	>20
Impurities	H_2O	ppm	< 20	<30	< 20
	HF		< 50	-	TBD
Purity of Each Component		%	≥ 99.99	>99.95	> 99.99
Vapor Pressure (25°C)		mm Hg	< 1	>10	> 10
Flashpoint		°C	> 100	<100	< 100
Lithium Salt Solubility		M	1	1	1
Cost		$/kg	< 10	-	TBD