Development of Large Format Lithium Ion Cells with Higher Energy Density

Principal Investigator: Dr. Fabio Albano
Global Cell Research and Development
XALT Energy LLC (formerly Dow Kokam LLC)

Annual Merit Review
DOE Vehicle Technologies Program
Washington, D.C.
June 16, 2014
Overview

Project Timeline

- Start date: Oct. 1, 2011
- End date: March 31, 2015
- Percent complete: ~81%

Project Goal/Barriers

Overall Project Goal:
To research, develop and demonstrate large format lithium ion cells with energy density > 500 Wh/L

Barriers addressed:
- Low energy density
- Cost
- Cycle life
- Safety/Abuse tolerance limitations

Project Budget

<table>
<thead>
<tr>
<th></th>
<th>DOE Share</th>
<th>$4,986,984</th>
</tr>
</thead>
<tbody>
<tr>
<td>XALT Share</td>
<td>$2,431,606</td>
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<td>Total Project Funding</td>
<td>$7,418,590</td>
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<td>Funding Shortfall:</td>
<td>$384,576</td>
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Partners

- **XALT Energy** – Project Lead
  - Cathode Materials and High Voltage Electrolytes

- **Wildcat Discovery Technologies**
  - Materials Characterization

- **Oak Ridge National Laboratory**
  - Testing/Characterization

- **Argonne National Laboratory**
  - Testing

- **UMKC**
  - Analytical Support
Project Objectives

• To research, develop, and demonstrate Li-ion battery cells that are capable of achieving an energy density of >500 Wh/L and a power density of >500 W/L while maintaining comparable performance standards in terms of cycle life (300-1000 cycles at 80% initial capacity), calendar life (5-10 years), and durable cell construction and design capable of being affordably mass produced.
Relevance to DOE targets

- XALT High Voltage Materials: **450~650 Wh/L** (design dependent)
- XALT High Capacity Materials: **500~750 Wh/L** (design dependent)
Approach/Strategy

• **Phase 1:** Mobilize Resources, Implement Project Management Plan, Institute Project Controls **(On-going)**

• **Phase 2:** Establish Model & Performance Baseline NMC/Graphite Cell, Establish Baseline Capacity For Cells, Install Equipment **(90% Complete)**

• **Phase 3:** Optimize High Voltage Cell Design and Finalize Materials Development, Scale Up High Voltage Cathode Material, Produce High Energy Interim Cells, Estimate Costs **(60% Complete)**

• **Phase 4:** Develop and Optimize High Capacity Materials and Cell Designs, Produce High Energy Interim Cells, Estimate Costs **(20% Complete)**

• **Phase 5:** Produce And Deliver Large Format Baseline and High Energy Cells **(Not Scheduled to Start Until November 2014)**

• **Phase 6:** Verify Achievement of Cost Goals and Develop Commercialization Plan **(20% Complete)**
## Project Milestones FY13

<table>
<thead>
<tr>
<th>Month/Year</th>
<th>Milestone or Go/No-Go Decision</th>
<th>Description</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>01/2013</td>
<td>Milestone</td>
<td>Final Model, Design, Cost and Testing of High Voltage System</td>
<td>Complete</td>
</tr>
<tr>
<td>03/2013</td>
<td>Milestone</td>
<td>Deliver Interim High Voltage Cells and Designs to DOE (&gt;500Wh/L)</td>
<td>Complete</td>
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<tr>
<td>07/2013</td>
<td>Milestone</td>
<td>Initial Model, Design, Cost and Testing of High Capacity Cell Design</td>
<td>Complete</td>
</tr>
<tr>
<td>01/2014</td>
<td>Milestone</td>
<td>Finalize Model, Design, Cost and Testing of High Capacity System</td>
<td>Complete</td>
</tr>
<tr>
<td>04/2014</td>
<td>Milestone</td>
<td>Deliver Interim High Capacity Cells and Designs to DOE (&gt;600Wh/L)</td>
<td>On Schedule</td>
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<tr>
<td>04/2014</td>
<td>Go/No-Go Decision</td>
<td>Select High Voltage or High Capacity or Both Systems for Scale up to Large Format Cells</td>
<td>On Schedule</td>
</tr>
<tr>
<td>04/2014</td>
<td>Milestone</td>
<td>Final Cost Comparison of High Energy Options Completed</td>
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- **NREL** – Testing/Characterization
- **Argonne National Laboratory** – Testing
- **UMKC** – Analytical Support
HV NMC performance and cycle life data

- > 300 cycles @ 1C/1C w/ capacity retention >80%
- > 600 Wh/L energy density
Safety Concerns: DSC at Full Charge – ORNL

- Differential Scanning Calorimetry (DSC) curves show safe operation at 4.4 V (full cell)
- Cells will be prepared for nail penetration tests
Responses to Previous Year Reviewer Comments

**Question 1: Approach to performing the work – the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.**

- "The reviewer stated that Dow Kokam now has a high-capacity anode, and it is developing a high-voltage cathode which still has issues (gas-generation during a cycle life test, though the cathode has apparently achieved 5V during cycling tests). It is also exploring high-capacity cathode materials, working with its partner Wildcat Discovery Technologies which is identifying the most promising materials that can optimize the desired cathode properties. The reviewer indicated that work seems to be at the stage of pursuing promising leads as of May 2013."
- "The reviewer stated that the selection of higher than graphite specific capacity and higher than NMC cathode is critical to reach 300 Wh/kg, 600 Wh/L for vehicle applications."
- "The reviewer commented being unclear on what is the project team’s performance goal is 370 Wh/L or greater than 500 Wh/L."

**RESPONSE:** XALT is planning to assess the scale up of the performance demonstrated in small cells to a large format cell targeting vehicle applications. The intention is to determine the manufacturability of a high capacity cell with an energy density of 500 Wh/L or greater as a step towards the programs production goals.

**Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.**

- "The team reported that its high-voltage cathode material has demonstrated an energy density of 340 Wh/L in 64X95-mm format full cells with graphite anode, which still falls short of the goal. The reviewer indicated that the high-capacity cathode materials are considered the much more experimental thrust of their project. This part of the project is contingent on the progress that project partner Wildcat Discovery Technologies is able to make in discovering suitable materials. The reviewer commented that Dr. Wu noted that because there had been a fire in Dow Kokam's cell testing facilities early on in the project, Dow Kokam had been granted a six-month extension to their project, and thus progress would lag as a result."
- "Issues are well defined, although the success of high voltage cathode (HVC) is a concern. The reviewer reported that multiple pathways to achieving the goals have been defined. What also lacks is the scalability effects of moving from the 2Ah cell to the large format cell design, and how that is to be inferred onto the goal chart. The reviewer noted that data was lacking in this presentation."
- "The reviewer stated that the energy density is only 370 Wh/L with continued gassing."
- "The reviewer indicated slow progress, only demonstrating 340 Wh/L using the high V cathode, and no cycle life data."

**RESPONSE:** XALT has since demonstrated 620 Wh/L in 8Ah cells and is planning to evaluate the scale up of the demonstrated performance in larger cells in Midland Battery Park in large format 51Ah and 75Ah cells.
Responses to Previous Year Reviewer Comments

• **Question 3: Collaboration and coordination with other institutions.**
  
  - “The reviewer reported that Dow Kokam is collaborating with Wildcat Discovery Technologies to identify high-capacity cathode materials, which is the heart of its experimental work here. Its other collaborations are with Oak Ridge National Lab for some materials characterization and failure mode analysis, and with a lab at the University of Missouri, Kansas City, for some analytical support.”
  
  - “The reviewer indicated that the right teams are working on the right sections. It is not clear however how project team members are interacting with each other to progress the overall project effort. This could result in an anode that is not fully compatible with the selected HCC/electrolyte couple.”
  
  - “The reviewer commented that the contribution of Wild Cat on selection of the appropriate high specific capacity anode and cathode is not very clear because they are not material suppliers and their selection is not optimized for energy and gassing.”
  
  - “The reviewer asked if there was any duplication of effort with other government funded high energy Li-ion cell.”

  **RESPONSE:** XALT has demonstrated that the HCA is fully compatible with HCC and HVC and has expanded the suppliers/collaborators pool to include BASF, Envia and Cabot. Cycle life and cost data is being generated. XALT anticipates that these last two deliverables would be a discriminant with respect to other projects.

• **Question 4: Proposed future research – the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways.**

  - “The reviewer reported that once some promising candidates for the high-capacity cathode material are identified and synthesized, these will be tested with the high-capacity anode in a cell. This full cell can then be measured to see how closely it achieves the goal of a higher-energy-density cell to achieve 500 Wh/L.”
  
  - “The reviewer noted that the development pathway is well defined, although specific barriers could have been better defined/listed in the presentation, and specific sub-tasks to close gaps listed.”
  
  - “The reviewer stated that the proposed future work is very good, but more focus is needed on the Si anode development. It is not clear that the difficulties of working with a Si anode are fully realized.”
  
  - “The reviewer stated that the high-capacity anode (HCA) should be either Si, SiO2, or Si/C composite, and high-capacity cathode (HCC) should be layered-layers or better capacity. Further, the reviewer observed that the High voltage cathode (HVC) needs a new electrolyte, and the development tasks are not very clear.”
  
  - “The reviewer felt more specifics were needed on how the project team will down-select between HVC and HCC.”

  **RESPONSE:** XALT has engaged XG Sciences as a collaborator on Silicon materials. The initial results seem promising pending optimization of cell design. HCA is a viable option for high energy cells manufacturing. We plan on expanding our options with respect to suppliers of the silicon-carbon composite materials.
Responses to Previous Year Reviewer Comments

- **Question 5:** Does this project support the overall DOE objectives of petroleum displacement? Why or why not?
  
  – "The reviewer stated that the increase in battery energy density is needed to make EVs an acceptable alternative to the gasoline powered vehicle. The objective of this project is to reach the DOE goals needed to offer that alternative."
  
  – "The reviewer noted that this project specifically targets the goals of improved energy density and low cost in large format cells, necessary to achieve longer term EV goals."
  
  – "The reviewer provided that XALT (ex. Dow Kokam) may be an automotive supplier with 300 Wh/kg and low cost cell or system supplier."

- **RESPONSE:** XALT understands that in order to achieve the overall DOE objectives of petroleum displacement, energy densities approaching 750 Wh/L and 300 Wh/kg are necessary in EV storage devices. XALT has demonstrated 620 Wh/L and 240 Wh/kg energy density in small scale 2Ah and 8Ah cells and is planning to demonstrate in the Midland Battery Park facility the scale up potential through the manufacture of 51Ah and 75Ah cells in BY3.

- **Question 6:** Resources: how sufficient are the resources for the project to achieve the stated milestones in a timely fashion?
  
  – "The reviewer reported that the project appears to be proceeding well on the funding that it has received so far."
  
  – "The reviewer indicated that resources are sufficient."
  
  – "The reviewer indicated no issues seen with respect to resource usage."

- **RESPONSE:** XALT feels that resources have been allocated appropriately and is very grateful for the support of DOE VT office; we plan on continuing improving the quality and reducing the cost of high energy density cells with a relevant format for EV applications and we encourage the DOE to reiterate their support for these projects;
Collaborations beyond VT program

- **Wildcat Discovery Technologies** – Dr. Bin Li
  - Screening of new HVC and HCC materials
  - Screening of dopants and additives to improve performance
  - Development of materials synthesis techniques

- **Oak Ridge National Laboratory** – Dr. David Wood
  - Materials characterization
  - Failure mode analysis

- **Argonne National Laboratory** – Dr. Ira Bloom
  - Cell performance testing

- **NREL** – Dr. G-H. Kim and Dr. A. Pesaran
  - Modeling parameters measurement
  - Characterization testing

- **UMKC** – Prof. Xiaobo Chen
  - Analytical support

- **DOD Title III** – Mr. Dilip Punatar
  - Materials deployment
  - Technology readiness evaluation
  - Scale up and cost model
• Worked with NREL to measure critical parameters
• Cell performance modeling will be employed to verify cell design parameters
Baseline Cells for evaluation by ANL

- Cells delivered to ANL 10/24/13
## Remaining Challenges and Technical Barriers

<table>
<thead>
<tr>
<th>Barrier - Challenge</th>
<th>Description</th>
<th>Mitigation Strategy</th>
</tr>
</thead>
<tbody>
<tr>
<td>HVC development</td>
<td>High voltage cathode did not perform as expected; cycle life was poor, gassing and conductivity issues;</td>
<td>explore more established HVC materials supplied by BASF, Envia and Cabot</td>
</tr>
<tr>
<td>HV electrolytes</td>
<td>Current electrolytes are not stable at HV and require further development of suitable additives or new generation electrolytes</td>
<td>continue present efforts on non-flammable electrolytes and leverage network to identify a suitable solution</td>
</tr>
<tr>
<td>HCA/HCC cyclability</td>
<td>Current cycle life meets the minimum 300 cycles requirements from DOE, however higher cycle life would make the use of this anode/cathode combination more compelling</td>
<td>deploy composite anode materials to minimize volume expansion</td>
</tr>
</tbody>
</table>
Future Work / Activities

• High Capacity Anode (HCA)
  – Fabricate and test 2-Ah full cells with HCA from supplier

• High Voltage Cathode (HVC)
  – Down-select alternative high voltage cathode material
  – Test improved CM1 when it is available
  – Combine HVC and HCA in 2-Ah format full cells, provide samples to ANL for testing

• High Capacity Cathode (HCC)
  – Contact commercial supplier for sample materials
  – Material characterization for physical and electrochemical properties

• Cost and business analysis
• Select the best solution and produce large format cells
Strategy for Deployment

• Demonstrate cell performance using manufacturing ready equipment in MBP
• Scale up 620 Wh/L cell prototypes to large format
• Build 24 large format (255x255 mm) cells
• Scale up synthesis of improved materials with goal to reduce manufacturing costs
• Develop bill of materials (BOM) and cost model specific to commercial and passenger EVs products
• Initial target markets, electric buses and/or fleet vehicles for product introduction
Project Summary

• Goal: To develop a large format lithium ion cell with energy density > 500 Wh/L

• Approach: Develop 2-Ah prismatic baseline cells using high voltage and high capacity cathodes, in parallel, with high capacity anodes

• Technical accomplishments in FY13:
  – Baseline cells completed, samples delivered to ANL
  – Si-Based anode material screened and selected, specific capacity >500 mAh/g demonstrated
  – High voltage cathode demonstrated 340 Wh/L in 2Ah – 64x95mm-format full cells with graphite anode
  – Development of high capacity cathode material initiated, currently achieved ~250 mAh/g, i.e. ~750Wh/L

*We gratefully acknowledge support for this project from the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies, Hybrid and Electric Systems of the U.S. Department of Energy under contract No. DE-EE0005384, subcontracts Nos. NFE-11-03678, TSA 14-587 and LS-111201A-MMW.*
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Technical Backup Slides

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Performance of 2-Ah Hand-Assembled Baseline Cells

Performance is the same or better than commercial 40 Ah cell
Performance of HV NMC / HCA Chemistry

- The combination of HV NMC and HCA seems promising
- Cell design optimization is underway
High Capacity Anode Development

• Si-based anodes provide high capacity as claimed
• Matching between anode and cathode is currently under investigation
• Charging conditions must be optimized
• XALT is testing full cells to reduce risk
High Capacity Cathode Development Status

<table>
<thead>
<tr>
<th>Metrics</th>
<th>Theoretical</th>
<th>HCC Baseline</th>
<th>HCC from Primary Screen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capacity (mAh/g)</td>
<td>288</td>
<td>240</td>
<td>267</td>
</tr>
<tr>
<td>Energy (Wh/kg)</td>
<td>1090</td>
<td>864</td>
<td>977</td>
</tr>
<tr>
<td>Rate Performance (% at 1C)</td>
<td>-</td>
<td>68</td>
<td>77</td>
</tr>
<tr>
<td>Reversible Capacity (%)</td>
<td>-</td>
<td>75</td>
<td>90</td>
</tr>
<tr>
<td>Full Cell Cycle Life (80% of Initial)</td>
<td>-</td>
<td>50</td>
<td>N/A</td>
</tr>
<tr>
<td>Stability</td>
<td>-</td>
<td>Air sensitive</td>
<td>Air stable</td>
</tr>
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Cycling rate: C/5
HCC//Li
2.5 – 4.9 V
30°C