

2. Energy Storage Technologies

Improving the batteries for electric drive vehicles, including hybrid electric (HEV) and plug-in electric (PEV) vehicles, is key to improving vehicles' economic, social, and environmental sustainability. In fact, transitioning to a light-duty fleet of HEVs and PEVs could reduce U.S. foreign oil dependence by 30-60% and greenhouse gas emissions by 30-45%, depending on the exact mix of technologies. While a number of electric drive vehicles are available on the market, further improvements in batteries could make them more affordable and convenient to consumers. In addition to light-duty vehicles, some heavy-duty manufacturers are also pursuing hybridization of medium and heavy-duty vehicles to improve fuel economy and reduce idling.

The Vehicle Technologies Office focuses on reducing the cost, volume, and weight of batteries, while simultaneously improving the vehicle batteries' performance (power, energy, and durability) and ability to tolerate abuse conditions. Reaching the Office's goals in these areas and commercializing advanced energy storage technologies will allow more people to purchase and use electric drive vehicles. It will also help the Department of Energy meet the EV Everywhere Grand Challenge of making the United States become the first nation in the world to produce plug-in electric vehicles that are as affordable for the average American family as today's gasoline-powered vehicles within the next 10 years.

The VTO pursues three major areas of research in batteries:

- **Exploratory Battery Materials Research:** Addresses fundamental issues of materials and electrochemical interactions associated with lithium and beyond-lithium batteries. This research attempts to develop new and promising materials, use advanced material models to predict the modes in which batteries fail, and employ scientific diagnostic tools and techniques to gain insight into why materials and systems fail. Building on these findings, it works to develop ways to mitigate those failures.
- **Applied Battery Research:** Focuses on optimizing next generation, high-energy lithium ion cells that incorporate new battery materials. The activity emphasizes identifying, diagnosing, and mitigating issues that negatively impact the performance and life of cells using advanced materials.
- **Advanced Battery Development, System Analysis, and Testing:** Focuses on the development of robust battery cells and modules to significantly reduce battery cost, increase life, and improve performance. This research aims to ensure these systems meet specific goals for particular vehicle applications.

This research builds upon decades of work that the Department of Energy has conducted in batteries and energy storage. Research supported by the Vehicle Technologies Office led to today's modern nickel metal hydride batteries, which nearly all first generation hybrid electric vehicles used. Similarly, the Office's research also helped develop the lithium-ion battery technology used in the Chevrolet Volt, the first commercially available plug-in hybrid electric vehicle. This technology is now being used in a variety of hybrid and plug-in electric vehicles coming on the market now and in the next few years, including the Ford Focus EV.

As described in the EV Everywhere Blueprint, the major goals of the Batteries and Energy Storage subprogram are by 2022 to:

- Reduce the production cost of an electric vehicle battery to a quarter of its current cost
- Halve the size of an electric vehicle battery
- Halve the weight of an electric vehicle battery

Achieving these goals would result in:

- Lowering battery cost from \$500/kwh to \$125/kwh
- Increasing density from 100 Wh/kg to 250 Wh/kg, 200 Wh/l to 400 Wh/l, and 400 W/kg to 2000 W/kg

Subprogram Feedback

The U.S. Department of Energy (DOE) received feedback on the overall technical subprogram areas presented during the 2014 Annual Merit Review (AMR). Each subprogram technical session was introduced with a presentation that provided an overview of subprogram goals and recent progress, followed by a series of detailed topic area project presentations.

The reviewers for a given subprogram area responded to a series of specific questions regarding the breadth, depth, and appropriateness of that DOE Vehicles Technologies Office (VTO) subprogram's activities. The subprogram overview questions are listed below, and it should be noted that no scoring metrics were applied. These questions were used for all VTO subprogram overviews.

Question 1: Was the program area, including overall strategy, adequately covered?

Question 2: Is there an appropriate balance between near- mid- and long-term research and development?

Question 3: Were important issues and challenges identified?

Question 4: Are plans identified for addressing issues and challenges?

Question 5: Was progress clearly benchmarked against the previous year?

Question 6: Are the projects in this technology area addressing the broad problems and barriers that the Vehicle Technologies Office (VTO) is trying to solve?

Question 7: Does the program area appear to be focused, well-managed, and effective in addressing VTO's needs?

Question 8: What are the key strengths and weaknesses of the projects in this program area? Do any of the projects stand out on either end of the spectrum?

Question 9: Do these projects represent novel and/or innovative ways to approach these barriers as appropriate?

Question 10: Has the program area engaged appropriate partners?

Question 11: Is the program area collaborating with them effectively?

Question 12: Are there any gaps in the portfolio for this technology area?

Question 13: Are there topics that are not being adequately addressed?

Question 14: Are there other areas that this program area should consider funding to meet overall programmatic goals?

Question 15: Can you recommend new ways to approach the barriers addressed by this program area?

Question 16: Are there any other suggestions to improve the effectiveness of this program area?

Responses to the subprogram overview questions are summarized in the following pages. Individual reviewer comments for each question are identified under the heading Reviewer 1, Reviewer 2, etc. Note that reviewer comments may be ordered differently; for example, for each specific subprogram overview presentation, the reviewer identified as Reviewer 1 in the first question may not be Reviewer 1 in the second question, etc.

Subprogram Overview Comments: David Howell (U.S. Department of Energy) – es000

Question 1: *Was the program area, including overall strategy, adequately covered?*

Reviewer 1:

The reviewer observed a very well-organized presentation that gives the audience an excellent overview of the U.S. Department of Energy's (DOE) overall strategy and the projects being worked on.

Reviewer 2:

The reviewer remarked that the program is directed at developing a new paradigm in transportation in the United States. The program is well funded to carry out the process and develop the new technology to assist U.S. car companies successfully compete in vehicle transportation market. The management is excellent and the plans and direction is superior. The reviewer added that given a little time, it will be a terrific advantage for the United States.

Reviewer 3:

The reviewer said yes, and found a comprehensive but detailed explanation of boundary conditions and program strategy.

Reviewer 4:

The reviewer remarked yes, although 30 minutes is obviously not enough to do anything but give a brief overview. The reviewer commented that the presentation was a bit low key. The reviewer wishes the program would do more to toot its horn. In particular, the reviewer thinks the knowledge gained in understanding the layered cathode material is outstanding, even if the answer is not what we would like, as it may be hard to fix the manganese (Mn) migration issue. This was, in this reviewer's view, a huge technical accomplishment and is really one of the great strengths of the national laboratories and the team approach taken.

The reviewer noted a good comparison of funding outlay versus gasoline saved; the 16:1 payback was impressive, as this reviewer was not actually expecting any payback until the technology was adopted more widely (2025 time-frame).

Reviewer 5:

The reviewer commented that while critical areas in battery systems were well covered, the reviewer strongly emphasized that the strategy was not clear, unless the areas studied constitute a strategy. In this reviewer's view, study materials, electrodes, cells and batteries are a list of areas, and not a strategy.

Question 2: *Is there an appropriate balance between near- mid- and long-term research and development?*

Reviewer 1:

The reviewer observed that there is excellent balance in the program. All aspects of vehicle technology relating to electric vehicles is being addressed and funding is at appropriate levels.

Reviewer 2:

The reviewer commented that the program is well structured and aligned to reasonable mid-term and long-term targets.

Reviewer 3:

The reviewer observed that the program was pretty well balanced based on the \$85 million dollar budget in the Office of Energy Efficiency and Renewable Energy (EERE). According to the reviewer, in a later talk it became clear there is program flow-through from the materials to the cell to the battery programs (e.g., Amprius).

Reviewer 4:

While the reviewer thought the overall distribution of funds is well aligned with overall objectives, the reviewer personally believed that further readjustment is possible. This reviewer thinks the biggest so-called bang for the buck will come out of the Exploratory Materials group. Advanced cell development should not get more than half the money that the Materials group gets. Thus, this reviewer's

suggestion is to lower both Advanced Cell Development and Battery Development work and redirect that money to the Materials group that will ultimately make the leapfrog we are all waiting for.

Reviewer 5:

This reviewer believed that there is an appropriate balance. The reviewer thought that most of the program seems directed at short- to mid-term goals in that while some goals are still very challenging, there is at least a clearly identified set of paths to success. It made sense to this reviewer to let programs such as Advanced Research Projects Agency - Energy (ARPA-E) and the Joint Center for Energy Storage Research (JCESR) handle some of the longer term quantum leaps in performance that may or may not ever pan out. The reviewer observed that some longer term work on lithium metal nodes is included in this program. While this reviewer is personally very skeptical that lithium metal batteries can ever be made safe enough for vehicle use (might be okay for utility applications), the program recognizes that this is the high risk/big reward part of this program. The reviewer observed a good target cost plus performance, although the reviewer expressed a little concern about the apparent short shrift given to safety. The reviewer pondered that maybe safety is viewed as not great but good enough, like consumer lithium-ion (Li-Ion). The reviewer was glad to see some work beyond Li-Ion, although the reviewer remains deeply skeptical about Li/O₂ and agreed that Li/air is a non-starter.

Question 3: Were important issues and challenges identified?**Reviewer 1:**

This reviewer agreed that important issues and challenges were identified.

Reviewer 2:

For this reviewer, the key issues of battery technology and the transfer of technology to appropriate automotive customers are being addressed. Both batteries and fuel cell technologies are supported. The reviewer remarked that it is clear that with the development of these new technologies, the corporate average fuel economy (CAFE) standard can be met in a timely fashion.

Reviewer 3:

The reviewer agreed yes, as a part of many of the accomplishments and the early material in the talk, the challenges were apparent.

Reviewer 4:

The reviewer noted that the key issue of increasing energy density and reducing costs were clearly addressed.

Reviewer 5:

The reviewer said yes. However, this reviewer thought there was too much emphasis on the battery pack and reducing manufacturing costs. The reviewer preferred that reducing manufacturing cost is best left to industry experts, as they are far better at this. The reviewer considered that maybe DOE has some unique game-changer approaches that might justify attention, but otherwise this reviewer would not expect the DOE program to address this. The reviewer guessed this gets back to whether the program is held accountable for cost goals or for advancing the state of the art so others can make a commercial success. The reviewer preferred the latter, but it seems the DOE programs are being judged by the former.

Question 4: Are plans identified for addressing issues and challenges?**Reviewer 1:**

The reviewer thought that plans were identified, in general.

Reviewer 2:

The reviewer observed that cost reduction is a driver for choosing program areas for part of future plans. This is a good way to pick areas because cost will decide in the end.

Reviewer 3:

The reviewer observed a comprehensive explanation of topics, projects and teams to address challenges.

Reviewer 4:

The reviewer found that the plans were clear and transparent. All of the needs are being addressed. For this reviewer, a viable, cost effective technology is essentially available today and with refinements will meet future needs. The only unanswered question is the cost of the new technologies. According to the reviewer, this ultimately will determine success or failure.

Reviewer 5:

The reviewer commented yes, although details were necessarily sparse as the time did not permit much detail. Most of the talk focused on what happened, which this reviewer thinks is appropriate for a Merit Review.

Question 5: Was progress clearly benchmarked against the previous year?**Reviewer 1:**

The reviewer commented yes, and elaborated it is clear that all areas are benchmarked for their timeliness and importance. Nothing has been left to chance.

Reviewer 2:

The reviewer concluded that the main achievements and progresses were demonstrated in different examples.

Reviewer 3:

The reviewer found that progress this year was well defined and last year's work was not "claimed" again; the new progress was the main focus of the talk.

Reviewer 4:

The reviewer commented that it was hard to do this in 30 minutes. The reviewer noted that the presentation mentioned some highlights and some metrics by year.

Reviewer 5:

Benchmarking of progress was not that apparent to this reviewer, in case it is the appropriate question for this presentation.

Question 6: Are the projects in this technology area addressing the broad problems and barriers that the Vehicle Technologies Office (VTO) is trying to solve?**Reviewer 1:**

The reviewer commented yes, and noted a broad attack on the major problems of durability, cost, and power or energy density.

Reviewer 2:

The reviewer agreed that projects are addressing broad problems and barriers.

Reviewer 3:

The reviewer commented that essential issues of electric transportation technology needs are being addressed and solutions developed. The reviewer observed that batteries seemed to be ahead of fuel cells today, but both are likely to be included in the transportation mix.

Reviewer 4:

The reviewer commented that projects are focused on main challenges.

Reviewer 5:

The reviewer commented yes.

Question 7: Does the program area appear to be focused, well-managed, and effective in addressing VTO's needs?**Reviewer 1:**

The reviewer found that due to good and effective project management, and by respectively directing the projects, the outcome is very good and addresses the Vehicle Technologies Office's (VTO) needs.

Reviewer 2:

The reviewer emphasized that yes, the program is focused on the objectives for electrified transportations and the program is versatile and complete. The only problem the reviewer observed is that U.S. car makers are slow to shift from gas powered engines to electrification.

Reviewer 3:

The reviewer commented yes, and referenced suggestions made in question two concerning a readjustment of funds.

Reviewer 4:

The reviewer commented that the program was certainly focused and well managed. What would help get DOE-origin batteries in vehicles is a plan where funds are focused where they are most needed, and particularly a quick refocus of resources to preferentially fund the areas where advancement is needed or where big progress is imminent. The reviewer thought the program has a plan and just did not express it as such.

Reviewer 5:

The reviewer commented yes, although this reviewer really got a better feel for what was actually being funded by looking at the other presentation rather than this presentation. The reviewer found that there was not enough time for the presenter to go over what is actually being funded in any detail.

Question 8: What are the key strengths and weaknesses of the projects in this program area? Do any of the projects stand out on either end of the spectrum?**Reviewer 1:**

For this reviewer, a key strength in this area is the strong effort to link different competence centers and make sure that there are common standards and testing protocols to make results comparable.

Reviewer 2:

The reviewer found that the program today is in a position to supply the needed technology to auto producers for them to produce a competitive electric vehicle for the marketplace. The advanced technology developed in the past five years places the electric car technology at the front worldwide. The U.S. automobile producers are holding back as they perceive a lack of interest in the part of general public. The reviewer commented that automobile producers also do not want to make the investment in new technology that overseas producers have recognized and are beginning to introduce. The reviewer cited Focused National Laboratory Project: Voltage Fade Mitigation of High Capacity Manganese Rich Layered-Layered Cathode Material as an outstanding project addressing both approach and results.

Reviewer 3:

The reviewer observed realism and honesty and appreciated that most solutions have their own set of challenges and that one can rarely get the full benefits of a new material/design indicated by test cells in a full cell. The reviewer noted the presentation avoided making many of the ridiculous claims that this reviewer often reads in technical and lay press. The reviewer acknowledged that the program team is using an extensive true team approach. For example, the work done to explain voltage fade of Argonne's layered-layered material involved a degree of teamwork often claimed but not usually realized in national laboratories or elsewhere. The reviewer noted a good selection of potential candidates, e.g., early recognition that Li/air was never going to meet goals even if we get it to work. The reviewer notes that basically, the program team has gone through the intellectual exercise of deciding ahead of time if we had it, would we really want it.

Reviewer 4:

The reviewer found that high capacity cathode and Si anode work are the program's strengths. The reviewer recommended that cell development, and focusing too much on cost reduction from processing points of view should be left primarily to manufacturers.

Reviewer 5:

The reviewer identified as strengths the wide range of programs and chemistries, so there are many chances to meet program goals. The reviewer observed knowledgeable staff and consultants, and good teams doing the work in most cases. The reviewer identified that a weakness is how some programs are carried after it is clear these programs are not going to make progress. The reviewer thought that the Energy Storage program would be more efficient if the program had an ability similar to Defense Advanced Research Projects Agency (DARPA) to end projects that are not going to make the progress needed or expected.

Question 9: Do these projects represent novel and/or innovative ways to approach these barriers as appropriate?**Reviewer 1:**

The reviewer said yes.

Reviewer 2:

The reviewer said yes and noted cutting edge techniques, analytical techniques, significant advances in modeling, and the program is working on a good selection of new approaches to boosting usable energy density.

Reviewer 3:

The reviewer said that in general, these projects do. While multiple projects with the same high risk/high payoff are okay, this reviewer's recommendation is to avoid redundancies as much as possible. The reviewer perceived that several projects appeared to have quite a bit of overlap and that one needs to justify such projects on very strong grounds.

Reviewer 4:

The reviewer said that the electrification of transportation is not a primary issue for the general public. The primary barriers are in the mind of the general public. The general public needs a comfort factor in choosing an EV over the traditional gas engine cars. The reviewer pointed out Tesla as a good example of the technology directed at the well-to-do public. According to the reviewer, the primary issue for the general public is cost. Today, the U.S. car manufacturers could produce an electric car for the general public at reasonable cost given an incentive. The reviewer noted that in the past the general public has insisted that EVs are expensive and ignored a smaller car that is common in most other countries.

Reviewer 5:

The reviewer commented that many projects were fairly advanced, or were innovations on well-known approaches. The reviewer said that appropriate techniques were used; one does not have to be truly novel to perform good work or use the right approach.

Question 10: Has the program area engaged appropriate partners?**Reviewer 1:**

The reviewer was very satisfied with partnership engagement.

Reviewer 2:

The reviewer observed that the program direction has covered all bases. Funding is available and the needs are being addressed. This reviewer does not know of any area that has not been addressed in an appropriate fashion.

Reviewer 3:

The reviewer observed that the project involves a number of worldwide recognized national laboratories or universities as well as technology leaders from industry.

Reviewer 4:

The reviewer responded yes. The reviewer observed that the program appeared to have a very good link to Vehicle Systems and Simulation (VSS) in terms of targets and metrics. This is a critical linkage in ensuring that if and when the program meets its targets, they actually are useful and will make a difference. The reviewer noted that it has always been hard to get meaningful partnerships with battery companies as these entities are so secretive and concerned about intellectual property (IP), and that this is not likely to change. The reviewer observed that the program managers seemed to do a lot of talking with interested parties up and down the supply chain, and this reviewer thought the program team put together a very reasonable program focused on near term must-have issues while also funding some longer term support projects. The reviewer noted good links to VTO and JCESR goals.

Reviewer 5:

The reviewer thought the mix of academia, labs, and companies seemed pretty good. The reviewer recommended that the program would benefit from collaboration with other programs in other countries.

Question 11: Is the program area collaborating with them effectively?**Reviewer 1:**

The reviewer remarked that everyone in the field was satisfied that the program was well directed and willingly contributes their time and effort on this important technology for the future.

Reviewer 2:

The reviewer said yes.

Reviewer 3:

The reviewer said that projects with effective collaborations were established in each program sub-area.

Reviewer 4:

The reviewer said that collaboration was the best that one could hope for.

Reviewer 5:

The reviewer said that the question's intent was unclear. However, according to this reviewer, the DOE staff works well with the contacted teams. If that was the question's intent, then this reviewer was in agreement.

Question 12: Are there any gaps in the portfolio for this technology area?**Reviewer 1:**

The reviewer saw no obvious gaps.

Reviewer 2:

In this reviewer's opinion, there are no gaps in the program portfolio.

Reviewer 3:

The reviewer commented that all relevant research areas are addressed.

Reviewer 4:

The reviewer observed no gaps, but had some concerns about dilution of effort. This reviewer was concerned about work directed at lowering costs that specifically includes advanced processing and battery manufacturing techniques. If this reviewer understood the scope of this work, it would seem to play much better into the strengths of industrial partners, equipment makers and engineering expertise. This reviewer thought the DOE national laboratories' strengths are significantly more in the chemistry area and cell analysis, battery data analysis, and determining failure modes. These are the areas where there are still major unknowns and obstacles, so this reviewer would think these people should remain focused on this area. The reviewer believed that it is a better fit and frankly a more important problem. In this reviewer's view, while the program team stated that the battery development work was often done with

partners, too much money was targeted at battery development. This reviewer would focus on materials and the 0.5-1 ampere-hour (Ah) cell. The reviewer opined that this is where the DOE national laboratories could really shine, especially in terms of understanding problems and evaluating new solutions. The reviewer stated that optimizing battery design for cost/performance is essential, but this reviewer did not believe the DOE programs needed to pay for this to get done. This reviewer recognizes that of course if given a directive, the program managers have little recourse but to follow them, but the reviewer perceives this is redirecting truly critical assets away from areas where assets can have the greatest impact.

Question 13: Are there topics that are not being adequately addressed?

Reviewer 1:

The reviewer concluded that all topics were being addressed. This reviewer was satisfied the program was complete and would be of great benefit to U.S. car companies and public buyers and users of electric propulsion.

Reviewer 2:

The reviewer would like to know under which portfolio non-lithium topics such as aqueous systems (sodium (Na)-based, for example) were addressed.

Reviewer 3:

The reviewer said moving from DOE to production in industry is not adequately addressed. The reviewer would like to know how to get U.S. automakers to pick it up and use it.

Reviewer 4:

This reviewer was not sure about next steps to stop Mn migration in layered-layered cathode. Hopefully, according to this reviewer, the other talks would cover this. The reviewer asked whether the layered-layered material, with coatings and other approaches to restrain fade issues other than voltage fade, was good enough for consumer applications where 150-500 high capacity cycles are fine. The reviewer said this might be a significantly easier and valuable entry point for this material than trying to jump straight into EVs.

Question 14: Are there other areas that this program area should consider funding to meet overall programmatic goals?

Reviewer 1:

This reviewer would like to see more basic research devoted to new class of electrolytes, especially from a non-flammability perspective.

Reviewer 2:

This reviewer indicated that safety seemed unrepresented and could not think of any others beyond this.

Reviewer 3:

The reviewer noted a barrier in that there are few filling stations for EVs as well as acknowledgement on the part of the general public that global warming is a key issue in the overall picture. Another problem is that EVs are more expensive than gas powered cars. The reviewer suggested that DOE may want to consider supporting electrification by initiating a \$5,000 instant payback on EVs.

Question 15: Can you recommend new ways to approach the barriers addressed by this program area?

Reviewer 1:

The reviewer commented that the program seems to be covering a wide range of opportunities.

Reviewer 2:

The reviewer commented that voltage fade is a hot issue and it has not been resolved to a satisfactory level despite elevated levels of funding. The reviewer observed that one aspect of the work that got low attention is doping. This reviewer was curious to know how a comprehensive approach affects the voltage fade.

Reviewer 3:

The reviewer commented that the main barrier to EVs is cost and range. The reviewer perceived that the program is mainly directed at the technology with cost the second. Today, this is the correct situation as the technology is just now reaching the point where cost can be addressed as well as technology. The reviewer commented that this is mainly a matter of educating the people on the advantages of EVs. The reviewer believed that a start would be making the public notice by establishing convenient charging stations at appropriate locations.

Reviewer 4:

The reviewer recommended advanced conceptual methods for controlling or designing batteries or electric powertrain systems, and battery control models.

Reviewer 5:

The reviewer suggested that the approach of a deep dive, such as the voltage fade project, can be transferred to other specific problems within the battery material research area.

Question 16: Are there any other suggestions to improve the effectiveness of this program area?**Reviewer 1:**

The reviewer found that overall, the program areas were well balanced requiring slight tweaking here and there as suggested above.

Reviewer 2:

The reviewer recommended setting up criteria for graduating from material programs to cell, to battery, and then to make them known to help researchers see where they should be aiming.

Reviewer 3:

The reviewer stated that the public needs to see visible evidence of the tremendous work that is being carried out and the world class capability of our scientists and engineers.

Reviewer 4:

The reviewer suggested focusing on cell chemistry and unit cell design. While scaling up large unit cells is okay, this reviewer did not think DOE should be expending so much energy on battery pack designs; the reviewer asked if others can do this (such as battery companies). The reviewer suggested that the focus should be on materials and cell design and understanding issues. Interfaces as usual are key, and DOE has some unique tools to study these. From talks later in the week, this reviewer was left unhappy about the status of the safety program and the cell tear down and analysis efforts. Based on what this reviewer had seen, both seemed pretty empirical and this reviewer questioned the usefulness of evaluating safety and doing tear downs without (in this reviewer's view) really understanding it. The reviewer recommended that both needed a shake up and a shift to a more fundamental approach.

Project Feedback

In this merit review activity, each reviewer was asked to respond to a series of questions, involving multiple-choice responses, expository responses where text comments were requested, and numeric score responses (*on a scale of 1.0 to 4.0*). In the pages that follow, the reviewer responses to each question for each project will be summarized: the multiple choice and numeric score questions will be presented in graph form for each project, and the expository text responses will be summarized in paragraph form for each question. A table presenting the average numeric score for each question for each project is presented below.

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Cell Analysis, Modeling, and Prototyping (CAMP) Facility Product	Andrew Jansen (Argonne National Laboratory)	2-16	3.67	3.50	3.83	3.08	3.53
Impact of Materials on Abuse Response	Christopher Orendorff (Sandia National Laboratories)	2-20	2.90	3.10	3.40	2.70	3.04
† High Capacity Composite Cathode Materials: New Synthesis Routes and Structures	Michael Thackeray (Argonne National Laboratory)	2-24	3.63	3.63	3.38	3.38	3.56
† High capacity, High-voltage Cathode Materials for Lithium-ion Batteries	Arumugam Manthiram (University of Texas at Austin)	2-27	3.25	3.25	3.50	3.13	3.27
† Design of High Performance, High Energy Cathode Materials	Marca Doeff (Lawrence Berkeley National Laboratory)	2-30	3.38	3.25	3.50	3.38	3.33
† First Principles Calculations of Existing and Novel Electrode Materials	Gerbrand Ceder (Massachusetts Institute of Technology)	2-33	3.67	3.33	3.00	3.17	3.35
† First Principles Calculations and NMR Spectroscopy of Electrode Materials	Clare Grey (University of Cambridge)	2-36	3.50	3.50	3.67	3.33	3.50
† Development of High Energy Cathode Materials	Jason Zhang (Pacific Northwest National Laboratory)	2-38	3.17	3.17	3.33	3.33	3.21
† Advanced in-situ Diagnostic Techniques for Battery Materials	Xiao-Qing Yang (Brookhaven National Laboratory)	2-41	3.33	3.17	3.17	3.00	3.19
† Nanoscale Heterostructures and Thermoplastic Resin Binders: Novel Li-ion Anode Systems	Prashant Kumta (University of Pittsburgh)	2-44	3.67	3.17	3.33	3.00	3.29
† Metal-based High Capacity Li-ion Anodes	Stanley Whittingham (Binghamton University-SUNY)	2-47	3.83	3.17	3.67	3.17	3.40
† Development of Electrolytes for Lithium-ion Batteries	Brett Lucht (University of Rhode Island)	2-49	3.30	3.20	3.50	3.20	3.26
† New Electrode Design for Ultrahigh Energy Density	Yet-Ming Chiang (Massachusetts Institute of Technology)	2-53	3.38	3.25	2.63	3.13	3.19
† Interfacial Processes in EES Systems Advanced Diagnostics	Robert Kostecki (Lawrence Berkeley National Laboratory)	2-56	2.83	2.83	3.00	3.00	2.88
† Predicting and Understanding Novel Electrode Materials From First-Principles	Kristin Persson (Lawrence Berkeley National Laboratory)	2-58	3.38	3.38	3.13	3.25	3.33
† Studies on High Energy Density Lithium Ion Electrodes	Jagjit Nanda (Oak Ridge National Laboratory)	2-61	3.38	3.25	3.50	3.25	3.31
Development of Computer-Aided Design Tools for Automotive Batteries	Steven Hartridge (CD-Adapco)	2-64	3.17	3.33	3.33	3.17	3.27

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Development of Computer-Aided Design Tools for Automotive Batteries	Taeyoung Han (General Motors LLC)	2-67	3.17	3.17	3.00	3.50	3.19
Development of Cell/Pack Level Models for Automotive Li-Ion Batteries with Experimental Validation	Christian Shaffer (EC-Power)	2-69	3.33	3.33	3.17	3.17	3.29
Open Architecture Software for CAEBAT	Sreekanth Pannala (Oak Ridge National Laboratory)	2-71	3.50	3.33	3.50	3.33	3.40
† Development of High Energy Density Lithium-Sulfur Cells	Donghai Wang (Pennsylvania State University)	2-74	3.20	3.00	2.80	3.00	3.03
† Silicon Nanostructure-based Technology for Next Generation Energy Storage	Ionel Stefan (Amprius)	2-78	3.20	3.40	2.70	2.90	3.20
† Development of Large Format Lithium Ion Cells with Higher Energy Density	Fabio Albano (XALT Energy)	2-82	2.80	2.70	3.00	2.90	2.79
† Modular Process Equipment for Low Cost Manufacturing of High Capacity Prismatic Li-Ion Cell Alloy Anodes	Sergey Lopatin (Applied Materials)	2-85	3.00	3.30	2.90	2.60	3.09
† High-Voltage Solid Polymer Batteries for Electric Drive Vehicles	Hany Eitouni (Seeo)	2-89	2.80	2.60	3.10	2.80	2.74
† Innovative Cell Materials and Designs for 300 Mile Range EVs	Yimin Zhu (Nanosys)	2-93	3.00	3.10	3.10	2.90	3.05
† High Energy Novel Cathode / Alloy Automotive Cell	Jagat Singh (3M)	2-96	3.30	3.40	3.20	3.20	3.33
† Utilization of UV or EB Curing Technology to Significantly Reduce Costs and VOCs in the Manufacture of Lithium-Ion Battery Electrodes	Gary Voelker (Miltec UV International)	2-99	3.25	2.75	3.75	3.25	3.06
† Significant Cost Improvement of Li-Ion Cells Through Non-NMP Electrode Coating, Direct Separator Coating, and Fast Formation Technologies	YK Son (Johnson Controls)	2-101	3.75	3.25	3.50	3.25	3.41
† Dry Process Electrode Fabrication	Mike Wixom (Navitas Systems)	2-103	3.00	2.75	3.00	3.00	2.88
† Stand-Alone Battery Thermal Management System	Brad Brodie (DENSO International America)	2-105	3.00	3.00	3.00	3.00	3.00
† Innovative Manufacturing and Materials for Low-Cost Lithium-Ion Batteries	Steve Carlson (Optodot Corporation)	2-107	2.83	2.83	3.17	3.00	2.90
† Novel Anode Materials	Jack Vaughey (Argonne National Laboratory)	2-110	3.50	2.83	3.33	2.67	3.04
† Development of High Capacity Anode Materials	Jason Zhang (Pacific Northwest National Laboratory)	2-112	3.67	3.33	3.50	3.17	3.42
† Atomic Layer Deposition for Stabilization of Amorphous Silicon Anodes	Chunmei Ban (National Renewable Energy Laboratory)	2-114	3.67	3.17	3.50	3.17	3.33
† Synthesis and Characterization of Polymer-Coated Layered SiOx-Graphene Nanocomposite Anodes	Donghai Wang (Pennsylvania State University)	2-116	3.67	3.17	3.33	3.17	3.31
† Wiring up Silicon Nanoparticles for High Performance Lithium-ion Battery Anodes	Yi Cui (Stanford University)	2-118	3.50	3.17	3.33	2.83	3.23

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Voltage Fade, an ABR Deep Dive Project: Status and Outcomes	Anthony Burrell (Argonne National Laboratory)	2-120	3.70	3.60	3.70	3.10	3.58
Overcoming Processing Cost Barriers of High-Performance Lithium-Ion Battery Electrodes	David Wood (Oak Ridge National Laboratory)	2-125	3.10	3.20	3.00	3.10	3.14
Roll-to-Roll Electrode Processing and Materials NDE for Advanced Lithium Secondary Batteries	David Wood (Oak Ridge National Laboratory)	2-129	2.92	2.83	3.00	2.92	2.89
Post-Test Analysis of Lithium-Ion Battery Materials at Argonne National Laboratory	Ira Bloom (Argonne National Laboratory)	2-133	2.83	2.50	3.17	1.83	2.58
Process Development and Scale-up of Advanced Cathode Materials	Greg Krumdick (Argonne National Laboratory)	2-137	3.50	3.40	3.60	3.10	3.41
Process Development and Scale-up of Advanced Electrolyte Materials	Greg Krumdick (Argonne National Laboratory)	2-141	3.25	3.50	3.50	3.25	3.41
† In situ Solvothermal Synthesis of Novel High Capacity Cathodes	Feng Wang (Brookhaven National Laboratory)	2-145	3.38	3.25	3.63	3.25	3.33
† Lithium Bearing Mixed Polyanion Glasses as Cathode Materials	Andrew Kercher (Oak Ridge National Laboratory)	2-148	3.25	2.88	3.63	3.13	3.09
NMR as A Tool for Understanding Voltage Fade in LMR-NMC	Baris Key (Argonne National Laboratory)	2-151	3.40	3.60	3.20	3.20	3.45
Electrochemical Characterization of Voltage Fade in LMR-NMC cells	Daniel Abraham (Argonne National Laboratory)	2-155	3.70	3.40	3.60	3.20	3.48
Electrochemical Modeling of LMR-NMC Electrodes	Anthony Burrell (Argonne National Laboratory)	2-159	3.00	2.80	3.40	3.00	2.95
Synthetic Approaches to Correcting Voltage Fade in LMR-NMC	Christopher Johnson (Argonne National Laboratory)	2-163	3.50	3.50	3.40	3.00	3.43
Atomic-Scale Models of LMR-NMC Materials	Hakim Iddir (Argonne National Laboratory)	2-166	3.30	3.30	3.30	3.10	3.28
Understanding Structural Changes in LMR-NMC Materials	Jason Croy (Argonne National Laboratory)	2-170	3.50	3.63	3.30	3.13	3.49
Significant Enhancement of Computational Efficiency in Nonlinear Multiscale Battery Model for Computer Aided Engineering	Gi-Heon Kim (National Renewable Energy Laboratory)	2-174	3.33	3.00	3.00	3.17	3.10
Coupled Hierarchical Models for Thermal, Mechanical, Electrical and Electrochemical Processes	Harry Moffat (Sandia National Laboratories)	2-177	3.00	2.83	2.83	2.83	2.88
Coupling of Mechanical Behavior of Cell Components to Electrochemical-Thermal Models for Computer Aided Engineering of Batteries Under Abuse	Ahmad Pesaran (National Renewable Energy Laboratory)	2-180	3.17	2.83	2.83	3.00	2.94
Efficient Safety and Degradation Modeling of Automotive Li-ion Cells and Pack	Christian Shaffer (EC-Power)	2-183	3.00	3.33	3.17	3.17	3.21
† Electrochemical Performance Testing	Ira Bloom (Argonne National Laboratory)	2-186	3.33	3.17	3.33	3.00	3.21
† INL Electrochemical Performance Testing	Jon Christophersen (Idaho National Laboratory)	2-189	3.50	3.33	3.67	3.33	3.42

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
† Battery Safety Testing	Christopher Orendorff (Sandia National Laboratories)	2-191	3.67	3.33	3.67	3.33	3.46
† Battery Thermal Characterization	Matthew Keyser (National Renewable Energy Laboratory)	2-194	3.75	3.25	3.75	3.25	3.44
† Advanced Battery Recycling	Steven Sloop (OnTo Technology)	2-196	3.50	3.50	3.50	3.25	3.47
† Real-time Metrology for Li-ion Battery R&D and Manufacturing	Jong Yoo (Applied Spectra)	2-198	3.00	2.50	3.00	3.00	2.75
Manufacturability Study and Scale-Up	Claus Daniel (Oak Ridge National Laboratory)	2-200	3.13	3.38	3.25	2.88	3.23
New High-Energy Electrochemical Couple for Automotive Applications	Khalil Amine (Argonne National Laboratory)	2-203	3.36	3.43	3.50	3.29	3.40
High Energy High Power Battery Exceeding PHEV-40 Requirements	Jane Rempel (TIAX)	2-207	2.67	2.58	2.25	2.58	2.56
Advanced High Energy Li-ion Cell for PHEV and EV Applications	Jagat Singh (3M)	2-211	3.21	3.14	3.50	2.93	3.18
High Energy Lithium Batteries for PHEVs	Subramanian Venkatachala (Envia)	2-215	3.20	3.00	3.30	3.10	3.10
High Energy, Long Cycle Life Lithium-ion Batteries for PHEV Applications	Donghai Wang (Pennsylvania State University)	2-219	3.13	2.88	3.13	3.00	2.98
High Energy Density Li-ion Cells for EVs Based on Novel, High Voltage Cathode Material Systems	Keith Kepler (Farasis)	2-222	3.30	3.00	3.40	3.10	3.14
† First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anodes	Perla Balbuena (Texas A&M University)	2-225	3.38	3.50	2.75	3.13	3.33
† Analysis of Film Formation Chemistry on Silicon Anodes by Advanced In Situ and Operando Vibrational Spectroscopy	Gabor Somorjai (University of California, Berkeley)	2-228	3.00	2.63	2.25	2.75	2.69
† Optimization of Ion Transport in High-Energy Composite Cathodes	Shirley Meng (University of California, San Diego)	2-231	3.33	3.00	2.67	3.00	3.04
† Daikin Advanced Lithium Ion Battery Technology — High Voltage Electrolyte	Ron Hendershot (Daikin America)	2-234	3.30	3.30	2.80	3.30	3.24
† Fluorinated Electrolyte for 5-V Li-Ion Chemistry	John Zhang (Argonne National Laboratory)	2-238	3.38	3.50	3.50	3.25	3.44
† Novel Non-Carbonate Based Electrolytes for Silicon Anodes	Dee Strand (Wildcat Discovery)	2-241	3.40	3.40	3.20	3.50	3.39
† Predicting Microstructure and Performance for Optimal Cell Fabrication	Dean Wheeler (Brigham Young University)	2-244	3.67	3.75	3.50	3.58	3.68
† A Combined Experimental and Modeling Approach for the Design of High Coulombic Efficiency Si Electrodes	Xingcheng Xiao (General Motors LLC)	2-248	3.17	3.33	3.33	3.17	3.27
† Electrode Architecture-Assembly of Battery Materials and Electrodes	Karim Zaghib (Hydro-Quebec)	2-250	3.70	3.50	3.60	3.50	3.56
† Advanced Binder for Electrode Materials	Gao Liu (Lawrence Berkeley National Laboratory)	2-253	3.75	3.63	3.75	3.50	3.66

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
† Fundamental Studies of Lithium-Sulfur Cell Chemistry	Nitash Balsara (Lawrence Berkeley National Laboratory)	2-256	3.60	3.70	3.60	3.60	3.65
† Design and Synthesis of Advanced High-Energy Cathode Materials	Guoying Chen (Lawrence Berkeley National Laboratory)	2-259	3.63	3.50	3.38	3.38	3.50
Microscopy Investigation on the Fading Mechanism of Electrode Materials	Chongmin Wang (Pacific Northwest National Laboratory)	2-262	3.38	3.13	3.00	3.00	3.16
Overall Average			3.32	3.20	3.27	3.11	3.22

Note: † denotes poster presentation.

Cell Analysis, Modeling, and Prototyping (CAMP) Facility Product: Andrew Jansen (Argonne National Laboratory) - es030

Reviewer Sample Size

A total of six reviewers evaluated this project.

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.

Reviewer 1:

The reviewer emphasized that the CAMP facility is critical to the battery research and development (R&D) community. The reviewer asserted that the facility plays an important and unique role among the national laboratory, industry, and academia for providing independent and critical validation analysis of newly developed battery materials.

Reviewer 2:

The reviewer highlighted that this research is critically-positioned between small lab-scale coin cells and large format production quantities. The reviewer voiced that, by positioning its significant capabilities in the valley of death (for scale-up), Argonne National Laboratory (ANL) is helping to accelerate the deployment of advanced battery materials.

Reviewer 3:

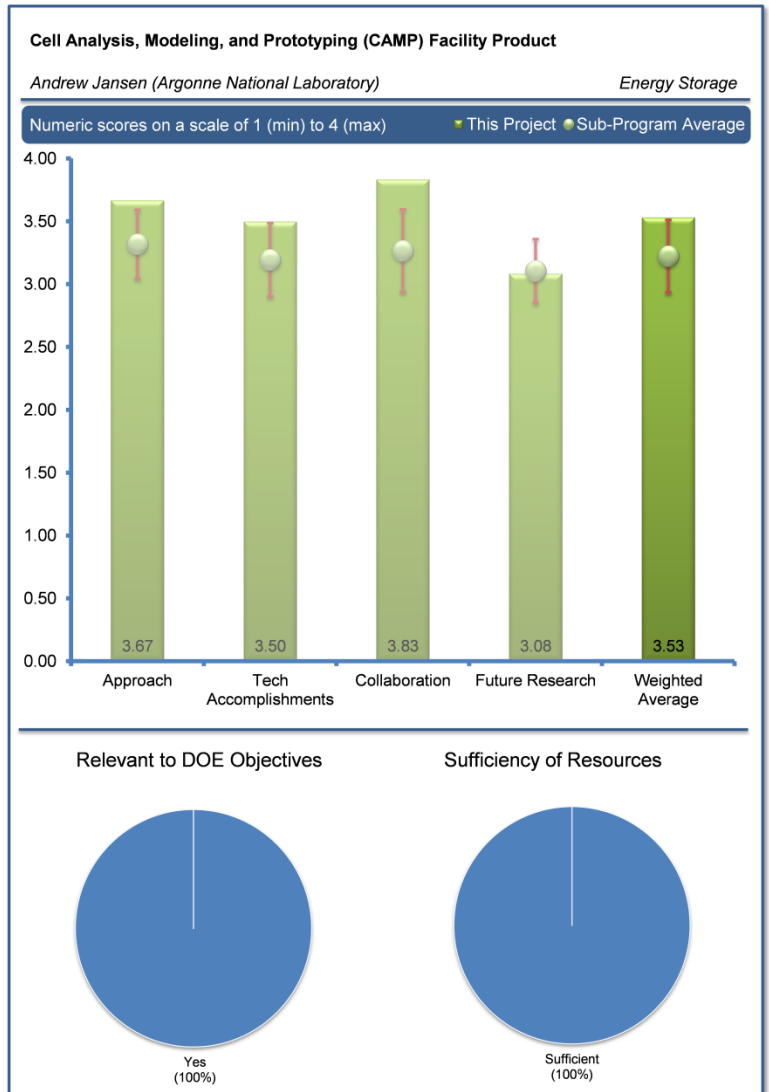
The reviewer reported that the ability to evaluate promising leads in larger format batteries is critical for establishing an effective commercialization roadmap for these concepts. The reviewer explained that this must be balanced with the difficulty of sufficiently large quantities of these new materials for further testing. The reviewer recognized that through a series of important examples, this work clearly demonstrated that the project facilities and staffing have struck an excellent balance between these issues and have addressed the barriers.

Reviewer 4:

The reviewer explained that the program is designed to provide a “pilot level” bridge manufacturing capability in the overall process of developing lithium-ion (Li-ion) cells with advanced designs. The reviewer stated that this is a critical step in the overall process of cell development, and if it is not available commercially, then this provides that capability. The reviewer cautioned that care should be taken as to determining the specific activity goals within this program. The reviewer also noted that cell concepts that have shown significant promise at smaller scale formats would be the candidate formats for development in this part of the development flow.

Reviewer 5:

The reviewer pointed out that the researchers have done an excellent job of getting as much expertise from industry and equipment makers (and maybe consultants) as one can to build a working system.



Reviewer 6:

The reviewer stated that the approach was useful and that it appeared to have met the objectives. However, the reviewer suggested that the formulation and material of choice was limited and could be more inclusive so that cause and effect could be established for mode of failure in silicon (Si) anodes.

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.**Reviewer 1:**

The reviewer explained that it was well-demonstrated that this laboratory could contribute substantially to the materials program by developing more effective formulation, better electrode manufacturing practices, and cell fabrication, which in-turn could facilitate proper and more realistic evaluation of new material including active materials, Si-anode, new electrolytes, and additives.

Reviewer 2:

The reviewer offered that the CAMP electrode library was a key accomplishment of this program. This reviewer also noted that the standardization effort was critical to moving the whole field forward. The reviewer also noted that the number of electrodes provided was significant. The reviewer would have appreciated greater metrics of the impact of this program upon other battery researchers. This reviewer described that the facility is best viewed as an enabler and not so much the pinnacle itself; recognition of this would better speak to its technical accomplishments and progress.

Reviewer 3:

The reviewer applauded that building a battery facility and getting “good” cells is quite a feat and the Principal Investigator (PI) deserves a lot of credit for this important task, even though it may be viewed as less glamorous than coming up with new “stuff.” The reviewer was also very impressed with the reproducibility they showed. The reviewer explained that the fact that the project is providing “standard” reproducible electrodes to other developers is extremely valuable for two reasons: 1) it enables anode, cathode and electrolyte developers to work on real, relevant systems without having to become experts in all aspects of cell design, and 2) by having standard materials, it can enable comparison between competing technologies on an “apples to apples” basis. For example, one could use this to rank Si/C approaches without the comparisons being plagued by issues related to the cathodes or electrolytes used. The reviewer summarized that this work helped one to pick real winners for future development.

Reviewer 4:

The reviewer stated that the technical accomplishments were focused on results related to scaling Si anode technology to this format level. It would have been helpful to the reviewer to review a summary of the coin cell work that occurred in this area, which would allow for a more informed review capability as to the additional knowledge that the larger format work provided.

Reviewer 5:

The reviewer described that the evaluations were focused on the U.S. Department of Energy (DOE) goals for high energy density, long cycle life, and cost reductions to enable further market penetration of battery-powered vehicles. The reviewer also explained that this work evaluated leading alternatives in Si anodes, and pointed to key performance issues that must be overcome with each candidate. The researchers characterized the role of electrolyte selection in addressing voltage fade in lithium (Li) and manganese (Mn) rich transition metal oxide (LMR-NCM), along with several other technologies. The reviewer commented that this work also shows that this team is versatile, and that they can accomplish outcomes in a wide variety of technologies that impact the development of better industrially-relevant battery performance and production.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer claimed that the collaborations were outstanding from their view. The reviewer especially liked the fact that in addition to get materials from others, that they also supply samples and even cross-check against other electrode manufacturers. The reviewer exclaimed that it would be hard to see how this could be improved.

Reviewer 2:

The reviewer reported that the collaborations within the laboratory and with external customers were very good.

Reviewer 3:

The reviewer indicated that the researchers have become an integral member of the battery research community working with a number of collaborators. The reviewer noted that the project team has also begun supplying a large number of electrodes to interested parties. The reviewer also explained that critical support of other DOE Office of Energy Efficiency and Renewable Energy-funded efforts as evidenced on Slide 17.

Reviewer 4:

The reviewer remarked that the program team has demonstrated a strong willingness to collaborate with a large number of universities, companies, and other national laboratories.

Reviewer 5:

The reviewer commented in the particular case of Si anode technology, that there are a wide range of materials under evaluation from a wide range of commercial developers. The reviewer stated that the collaboration presented was quite competent. The reviewer explained that it is simply a fact of the field that there will be a wide range of materials under development that may not represent the slice of technology provided by any one entity.

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.

Reviewer 1:

The reviewer suggested that as the project comes to an end, it would be valuable to document and publish the findings in open literature to benefit the battery R&D community.

Reviewer 2:

The reviewer noted that the plans to look at changes that can be made to get Si/C to work are critical. The reviewer cautioned, however, that this needs a very thorough and disciplined approach and needs a grand plan for this agreed upon by the major stakeholders. The reviewer warned, however, that the group must avoid just picking a few hot candidates and testing them one at a time, which far too often is the case in academic and government lab work, for various, somewhat understandable reasons. The reviewer observed that several of the approaches are likely to have very strong interactions; both positive and negative. The reviewer proposed that the team has to plan some designed experiments to look at interactions/synergies among stabilization efforts being pursued by the various groups and not treat it as a straight A versus B competition; this applies to both anode and cathode improvements and interactions between anode and cathode stabilizations are likely. The reviewer offered that planning such work is not trivial, but often this is where the most value can be added.

Reviewer 3:

The reviewer remarked that there seemed to be a large number of milestones still to be completed before the end of Fiscal Year (FY) 2014. The reviewer also pointed out that there does not seem to be a pathway to keep this unique and important facility working. The reviewer was very interested in the results of the work breaking down the three major contributors to energy fade (i.e., voltage fade, impedance rise, and capacity fade).

Reviewer 4:

The reviewer acknowledged that the capability demonstrated by the group is quite good, and quite valuable. The reviewer suggested that the process for defining what the high priority programs could be more transparent, which may or may not be in the purview of this specific group.

Reviewer 5:

The reviewer observed that the scope of objectives was very broad and criticized that they could not see any clear decision-making plan or critical-path analysis. The reviewer indicated that both should help with streamlining of activities toward obtaining desired results.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer agreed that this program is critical to generate reliable data on new materials and approaches and provides an invaluable service to the community. The reviewer specified that this work forms a solid foundation on which the rest of the community can build.

Reviewer 2:

The reviewer stated that this project would help the domestic industry to quickly streamline their processes for making better and more cost-competitive materials for Li-ion batteries.

Reviewer 3:

The reviewer affirmed that scale-up activities were important for ensuring that advanced battery materials make it from the bench to the consumer and ultimately displace petroleum.

Reviewer 4:

The reviewer indicated that this was a necessary capability in the overall development of advanced battery chemistries.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer said the allocation of resources appeared to be adequate, although the details were not discussed. The reviewer stated that it would be interesting to know where the bottleneck is, and how it can be resolved.

Reviewer 2:

It was unclear to the reviewer if the large amount of funds were spent on setting up this facility (funds considered sufficient), or not (funds considered excessive). The reviewer also would have liked to see a longer-term plan for this core funded facility.

Reviewer 3:

The reviewer stated that no information was presented to indicate that project areas would go unaddressed because resources were limited.

Impact of Materials on Abuse Response: Chris Orendorff (Sandia National Laboratories) - es036

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer agreed that the global objectives were in line with other efforts and approaches. However, the reviewer suggested that the detailed objectives can be refined to identify the chain-of-events that could result in cell failure or compromised safety. The reviewer proposed that it might be possible, at least in theory, that safety concerns could be alleviated by interrupting the chain-of-events rather than changing active materials.

Reviewer 2:

The reviewer agreed that the production of more robust batteries will accelerate their commercial deployment. The goal of this team was to alter existing chemistries to improve safety without compromising performance. There was a strong desire by the reviewer for more quantitative metrics on abuse tolerance. If not, the reviewer asked what the key thresholds are that represent a robust battery system. The reviewer agreed that this project is made up of good science, it just needs to be better applied to relate directly back to batteries, especially as they are used in vehicles.

Reviewer 3:

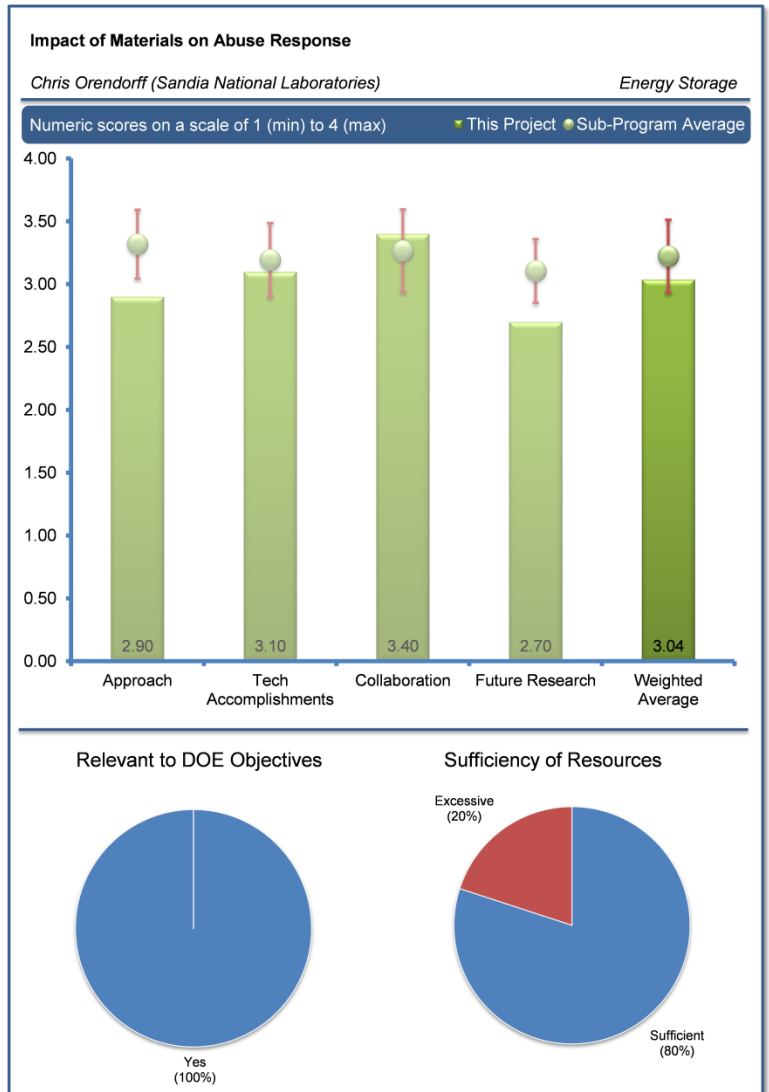
The reviewer stated that the program demonstrated methods to characterize abuse with both quantitative and qualitative outcomes. The reviewer explained that the methods tended to be more materials-based, with limited chemical insight developed thus far.

Reviewer 4:

The reviewer stated that the overall approach was okay, but this person was a little concerned about the low capacity of the project team's 18650 cells – presumably these cells had a much higher electrolyte to solids ratio than “real” cells and burning electrolyte was apparently the biggest source of heat in these events. The reviewer thought that the researchers were looking at the right variables, but the reviewer remained concerned about the relevance of the 18650 test vehicle to actual vehicle batteries. Typically, in such cells, the role of the vent in ensuring safety can be very important and the project had not really addressed this level of complexity yet. The reviewer would like to know whether venting really helped cell safety, or if it actually made it worse (may depend on whether the expelled electrolyte catches fire which may in turn depend on spark/ignition sources). The reviewer recognized that this was not easy.

Reviewer 5:

The reviewer said that it seems that only thermal runaway is addressed in this project. It was unclear to the reviewer whether industry-accepted standard test procedures were used for the thermal runaway tests. It was also unclear whether the results from the project could



be used to help develop Li-ion cells and batteries that are abuse-tolerant under more realistic conditions, such as under the influence of multiple factors (e.g., mechanical damage, air exposure, and thermal runaway) that may occur simultaneously. The reviewer also voiced that the project does not address aged battery cells that may have completely different abuse tolerance. It was unclear to the reviewer how statistical analysis was used for abuse failures that are usually random and low-probability events.

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.

Reviewer 1:

The reviewer stated that it was well-demonstrated that this laboratory could contribute substantially to the materials selection program to address battery safety. However, the reviewer proposed that a more systematic approach to establishing a clear and unambiguous chain of events that could lead to battery failure would benefit this program.

Reviewer 2:

The reviewer commented that there is only one journal publication listed together with four conference presentations (Slide 18). The project person offered that it would be valuable to the R&D community if the results from the project can be found in archival journals.

Reviewer 3:

The reviewer stated that the PI showed a number of key successes in raising autoignition and thermal runaway temperatures and lowering the corresponding enthalpy. However, without a clear baseline it was difficult to put this research into context. The reviewer indicated that the key takeaways did not translate back well to the overall project objectives.

Reviewer 4:

The reviewer stated that this program described the challenges in assessing the contribution of Si anode to thermal abuse, but has yet to clarify the causes of the variation, nor the significance of any additional concerns over graphite. In contrast, the reviewer highlighted the significant improvements demonstrated for LiMPO₄-coated NMC show the soundness of this program's approach and its ability to deliver important accomplishments. Similarly, the evaluation of novel electrolyte components that brings FRION effectiveness into question and qualifies the safety benefits of the LiF/ABA against battery performance trade-offs are significant accomplishments. The reviewer commented that these examples demonstrate the promise and perhaps some limitations to characterizing abuse.

Reviewer 5:

The reviewer affirmed that the researchers have added to some of the fundamental knowledge on Si anodes; however the reviewer did not think the lower onset temperatures was a very positive feature for this system.

It remained unclear to this person whether it was more important to delay thermal runaway or to have less heat produced if it goes off. Delaying thermal runaway may render a cell more abuse tolerant, but may not stop propagation or the scale of any thermal runaway that does occur. Having a lower heat output may help tame the violence of a runaway (and propagation), but may not reduce the tendency of cells to cook off in the first place. The reviewer supposed that both are important, but thought that TIAX's modeling work presented a while back suggested that once the onset temperature of the anode is reached, thermal runaway in large cells can proceed very quickly regardless of cathode material. If true, more emphasis may be warranted for avoiding the start of an event rather than trying to tame it once it has started (i.e., onset temperature may be more important than energy).

The reviewer also proposed that the role of cell vents seemed to warrant more consideration. The reviewer asked if the venting of a cell early enough caused the cell to shut down enough to stop thermal runaway. If so, the very high pressures seen by some of the Si anodes could actually be an advantage. Also, the reviewer wanted to know if venting was inherently going to cause a fire in the absence of ignition sources, and explained that Sandia's use of a sparking station to set electrolyte vapors alight is a worst-case scenario. The reviewer asked if standard electrolyte vapors will always tend to ignite in a real thermal runaway for a car battery pack. Pouch cells would also have very low vent/burst pressure and may pose different, not necessarily better, safety characteristics.

The reviewer asserted that the link between what SNL was measuring and safety in electric vehicles (EV), hybrid- electric vehicles (HEV), and plug-in hybrid- electric vehicles (PHEV) cells seemed weak. The reviewer explained that size and scale are so critical to

this runaway issue that more work on larger cells was needed. The reviewer agreed that these were hard questions to answer, but this person thought that it should be attacked; it gets at the whole validity of the project team's work. Finally, the reviewer criticized that the amount of work done does not in the reviewer's view seem to be very large. The reviewer asked if the researchers could not pick up the pace a bit.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer reinforced that the partnering to get commercial materials and the collaboration had been a critical element of the work in this project. The reviewer reported that there had been a number of successfully coordinated efforts with project successes. The reviewer was encouraged by the substantial industry engagement.

Reviewer 2:

The reviewer affirmed that collaborations within the laboratory and with external customers were very good. The reviewer proposed that collaboration also can be extended to development of new materials based on identifying the weak link in the battery.

Reviewer 3:

The reviewer explained that although a limited number of collaborations were described, they were well-chosen to address the goals of this program. The reviewer claimed that the accomplishments of the program are likely to attract additional collaborations with programs that are targeting new concepts for improving battery safety.

Reviewer 4:

The reviewer described that the researchers were getting samples and presumably giving feedback on results to partners, which seemed to be okay.

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.

Reviewer 1:

The reviewer agreed that the overall objectives were in line with the needs of industry. The reviewer suggested that it would be beneficial also to establish the chain of events that could lead to the failure and to identify the weak link in Li-ion battery safety. The reviewer summarized elements from the summary: 1) fielding the most inherently safe chemistries and designs can help address the challenges in scaling-up Li-ion, and 2) materials choices can be made to improve the inherent safety of Li-ion cells. Based on this logic one can conclude that gasoline should not be used in automobiles; however, proper engineering design and suitable material of choice made it possible.

Reviewer 2:

The reviewer remarked that most of the proposed future work, which seems to be a continuation of the current course, is sufficient. The reviewer indicated that the modeling/statistical analysis of the data will be key to generating usable information on how to improve abuse tolerances. This person expected there to be a greater focus on developing recommendations/guidelines for other researchers.

Reviewer 3:

The reviewer simply stated that the future work was focused on continuing current activities.

Reviewer 4:

The reviewer thought that the researchers' plans were fine as far as they go, but would have also liked to see more work done to ensure the work was truly relevant. The reviewer also commented that there was little actual chemistry in the presentation, so the reviewer was glad to see some analysis of the vented gases included in the future work.

Reviewer 5:

It was unclear to the reviewer whether the large number of tasks listed under proposed future work could be accomplished in the remaining few months of the project.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer stated that this project would help the domestic industry to quickly streamline their processes for making safer and more cost-competitive materials for Li-ion batteries.

Reviewer 2:

The reviewer asserted that consumer fear of catastrophic battery failure was a drawback. Inherently safer battery designs limit this risk and accelerate deployment.

Reviewer 3:

The reviewer remarked that battery safety was an important and highly-publicized concern for the use of batteries in transportation. Therefore, methods to characterize safety, and search for improvements were very relevant to transition the consumer away from petroleum-based transportation.

Reviewer 4:

The reviewer reported that safety was obviously critical for Li-ion batteries, and appeared to be especially troublesome for large, high-energy and high-power battery packs needed to meet DOE goals.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer agreed that the allocation of resources appeared to be adequate, although the details were not discussed. It would be interesting to this person to know where the bottleneck was and how it could be resolved.

Reviewer 2:

The reviewer indicated that the program did not describe work that could not be completed due to insufficient resources.

Reviewer 3:

The reviewer commented that the resources seemed to be sufficient, but criticized that the amount of work done seemed to be rather modest. Currently, the bang for the buck was not there for this person.

Reviewer 4:

The reviewer warned that the invested funds, particularly on the abuse evaluation side, seemed to be quite high for the quantity and quality of research data generated.

High Capacity Composite Cathode Materials: New Synthesis Routes and Structures: Michael Thackeray (Argonne National Laboratory) - es049

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer commented that among the approaches pursued that entailing tailoring of the bulk structure, the integration of stabilizing spinel, etc., appeared to be of the most benefit. The reviewer, however, was doubtful about the efficacy of approaches using surface modification to yield any fundamental breakthroughs to resolve the issues of life and voltage fade.

Reviewer 2:

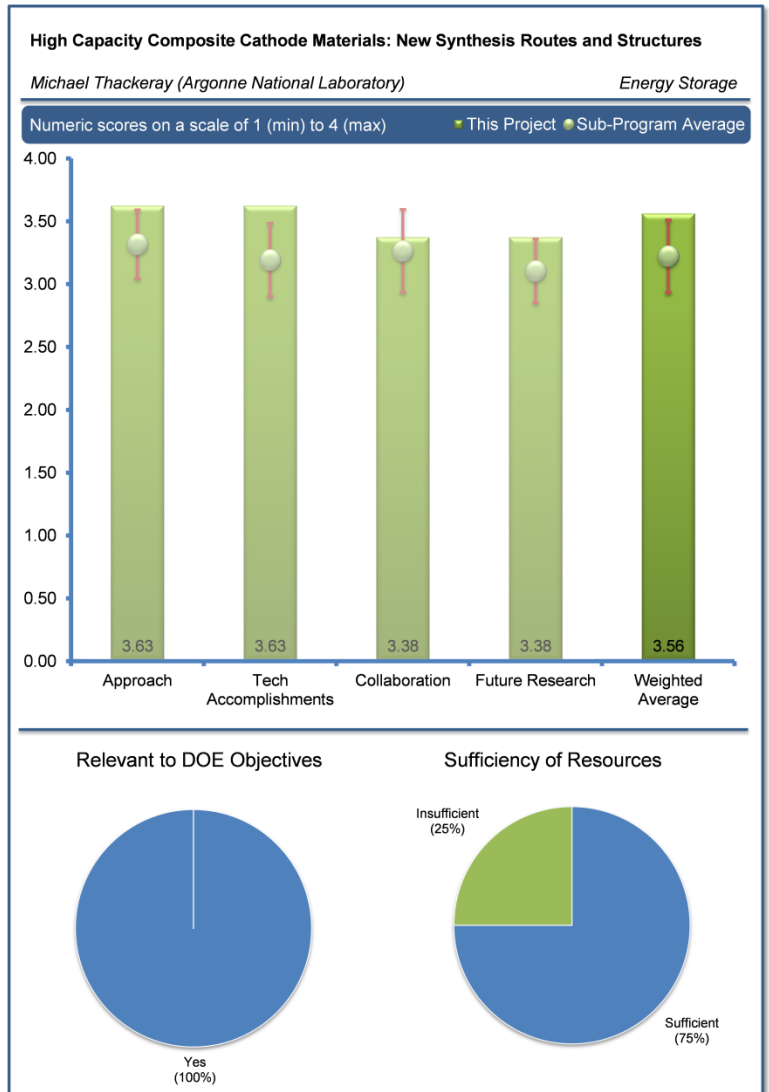
The reviewer applauded the excellent approach, also indicating that the availability of a battery with high energy is essential to the success of the program.

Reviewer 3:

The reviewer explained that the project objective is to stabilize the nanocomposite structures of Li_2MnO_3 and LiMO_2 layered structures from the formation of the pseudo-spinel phase that contributes to its voltage fade upon cycling. The reviewer explained that the adopted approach includes developing integrated structures incorporating a spinel phase (for a layered-layered spinel composite [LLC]) with improved processing methods and further stabilizing these materials with suitable surface coatings. The reviewer confirmed that this project thus addresses one of the key performance barriers of the LMR-LLC cathodes, by adopting a viable approach and is well-integrated with the other efforts in understanding/mitigating the voltage fade. One question remained in the reviewer's mind, however, with the incorporation of the low-capacity (and low-voltage) spinel phase, if the LMR-LLC materials with spinel components compete well with simple surface-treated nickel (Ni)-rich layered cathodes operating at higher voltages.

Reviewer 4:

The reviewer commented that this is a good fundamental research to understand the phase transition mechanisms.



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.**Reviewer 1:**

The reviewer confirmed that the approach to identify and develop a suitable battery for EVs is key. The reviewer explained that Dr. Thackeray has a long history of success in developing battery systems, from those for EVs as well as to power portable electronics. The reviewer recognized that the PI has been a key performer at ANL for many years.

Reviewer 2:

The reviewer described that impressive progress had been made in understanding the processes contributing to the voltage fade of LMR-LLC materials and in the design and verification of new layered-layered-spinel composite structures. The reviewer highlighted that some of the significant findings included the following: stabilization of the Li_2MnO_3 with the incorporation of Ni^{2+} incorporation, even with high Li_2MnO_3 proportions; and development of synthetic technique for the structurally integrated layered-layered-spinel composites, which were confirmed through X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), and electrochemical cycling. Further, the reviewer mentioned that some good publications had emerged from this project.

Reviewer 3:

The reviewer explained that the research has focused on understanding of what leads the degradation of Li_2MnO_3 and LiMnNiO_4 cathode using conventional electrochemical and XRD methods.

Reviewer 4:

The reviewer noted that the data showing the effect of stabilization of the Li_2MnO_3 structure looks promising. However, the reviewer cautioned that there are only little data to support the hypothesis that this approach will eliminate all the major issues that plague this LMR cathode (e.g., life especially at high temperatures, voltage fade, and gassing).

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer stated that all of the pertinent laboratories were involved in this collaboration.

Reviewer 2:

The reviewer observed that there are good collaborations with several researchers from the “voltage fade” team. The reviewer stated that it was probably the appropriate time to collaborate closely with industry (i.e., BASF, Toda, LG, and Envia) for further verification of the layered-layered spinel composite material in the industrial environment.

Reviewer 3:

The reviewer acknowledged that Dr. Thackeray is a leading proponent for battery-powered transportation. The reviewer indicated that the cathode materials, developed for portable electronics, are being used in most portable computers. The person recognized that Dr. Thackeray is a team performer and shares thoughts willingly and spontaneously. The PI’s stature in the industry makes it easy for him to cooperate with anyone in the industry and is always ready to cooperate.

Reviewer 4:

The reviewer was unsure if there was any evidence of collaboration outside of ANL so far.

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.**Reviewer 1:**

The reviewer agreed that the work was definitely focused on resolving the key issues, but suggested to bring about bulk stability of the material in the course of life.

Reviewer 2:

The reviewer reported that the approach used by Dr. Thackeray was based on sound ground. The reviewer pointed out that the PI had claimed several awards for work including the Technology Award from the International Battery Association. The reviewer also commented that the materials will find use in advanced vehicle propulsion.

Reviewer 3:

The reviewer explained that the proposed future research will continue the development of LMR-LLC cathodes to achieve high capacities combined with adequate stability on cycling. Composite structures with low Li_2MnO_3 -content composite structures, with and without stabilizing spinel components, look promising. The reviewer agreed that basic studies related to the charge ordering and magnesium (Mg) mobility are useful in designing stable composite compositions which may be further protected with surface coatings to mitigate voltage fade and realize high energies. The reviewer emphasized that it is, however, important to demonstrate that these approaches also address the other limitations of the LMR-LLC compounds, which are yet to be successful in an industrial environment (e.g., with high cathode loadings and in full cells) due to their poor power characteristics and cycle life. The reviewer concluded by stating that voltage fade appears to be a minor component of the energy fade upon cycling.

Reviewer 4:

The reviewer commented that the proposed future research is relatively focused, but this person was unsure of how the coating on the particles could stabilize the phase transition inside particles.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer agreed that this project was highly-relevant to DOE's overall objective of petroleum displacement by advancing the next generation high capacity cathode chemistry for low-cost and long-life batteries.

Reviewer 2:

The reviewer stated that the development of batteries to service electric vehicles was an essential part of the DOE assignment.

Reviewer 3:

The reviewer explained that the low specific energies and high costs of Li-ion batteries were serious impediments to their widespread adoption in vehicles. The reviewer suggested that LMR-LLC cathode materials were promising, both from an energy and cost perspective, but were hampered by issues such as voltage fade and hysteresis. According to the reviewer, it is essential to have a fundamental understanding of these phenomena to mitigate these issues and to develop stable structures, as was being done in the present project.

Reviewer 4:

The reviewer commented that the project would develop high capacity high-voltage cathode for Li-ion batteries.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer simply stated that the funding was appropriate.

Reviewer 2:

The reviewer indicated that the resources were adequate for the scope of the project.

High capacity, High-voltage Cathode Materials for Lithium-ion Batteries: Arumugam Manthiram (University of Texas at Austin) - es051

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer commented that the approach is very sound and that the work has developed high-performance spinels and polyanion cathode materials such as phosphates and silicates. The reviewer also reported that a fundamental understanding of the structure and performance with good performance and high-voltage was developed. The reviewer also explained that low temperature synthesis of these materials was developed as the use of graphene as a conductive diluent. The reviewer reported that solid-state, high-energy ball milling, and solution-based synthesis approaches were used along with advanced chemical, structural, and surface characterizations. The researchers also performed an in-depth electrochemical evaluation including impedance analysis to develop an understanding of the structure-property-performance relationships.

Reviewer 2:

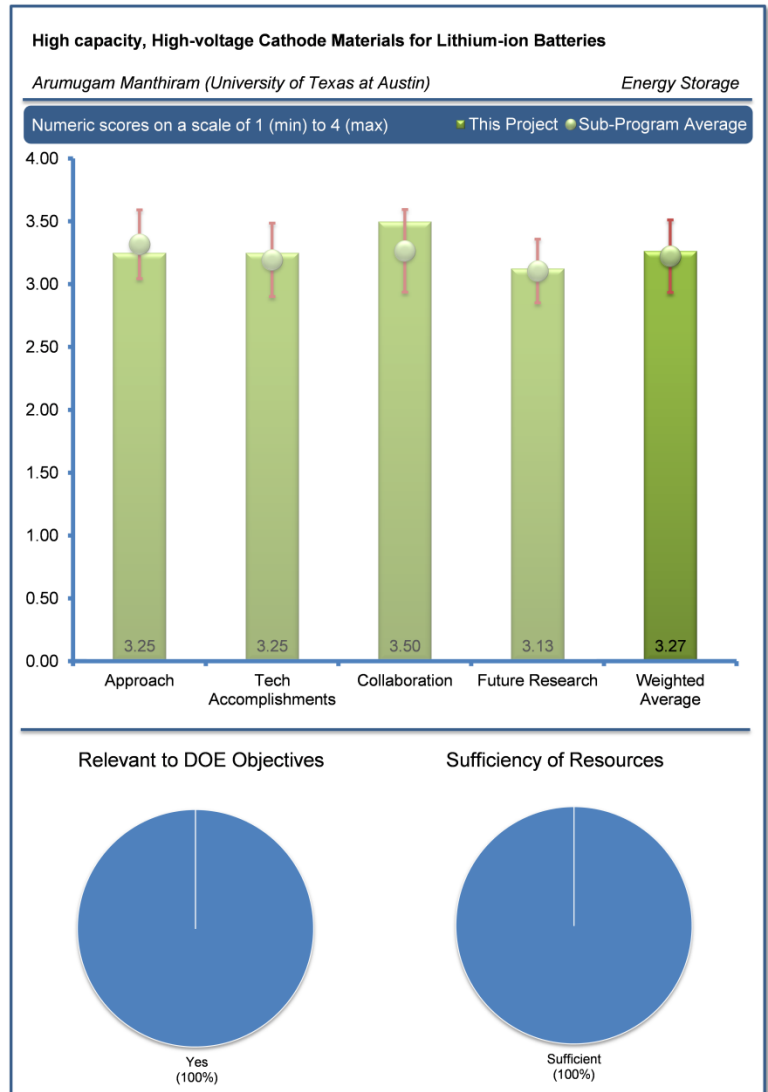
The reviewer described that the project objective here is to develop new polyanion cathodes with high specific energy for Li-ion batteries, specifically based on high-energy density phosphate and silicate cathodes exhibiting multi-electron redox process, and to gain a fundamental understanding of their structure-composition-performance relationships. The reviewer reported that three types of cathodes were being developed including the three polymorphs of LiVOPO_4 wherein two Li ions can intercalate, and nanostructured phosphate and silicate cathodes with either graphene inclusions of aliovalent metal dopings for enhanced conductivities and performance. The project person also described that low-temperature synthesis methods are being developed for these cathodes ionic and electronic transport. Using detailed chemical, structural and surface characterization; the electrochemical performance was correlated with the materials' structure and property. The reviewer indicated that this approach was proving to be feasible for the development of new cathode materials.

Reviewer 3:

The reviewer reported that microwave-assisted synthesis was used to synthesize LiVOPO_4 , and chemical and electrochemical lithiation methods were used to insert additional Li into the cathode structure.

Reviewer 4:

The reviewer agreed that the approaches will definitely lead to a better understanding of these classes of (potentially) stable cathode materials. The reviewer, however, was not sure though whether any of them would be practically useful.



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.**Reviewer 1:**

The reviewer commented that the work established a new method for identifying new cathode materials for vehicle applications.

Reviewer 2:

The reviewer described that several cathode materials with multi-electron redox processes were being developed and that the initial results were encouraging. For example, high capacities of approximately 220 mAh/g were demonstrated in the three polymorphs of LiVOPO₄. High capacities of 155 mAh/g were realized with aliovalent substitution of V³⁺ for Mn²⁺ in LiMnPO₄. Finally, the reviewer noted that the nanostructured Li₂MnSiO₄-carbon composite cathodes synthesized with a hard-template approach exhibit stable cycling at high rates (1C rate) with a capacity of 100 mAh/g. The reviewer cautioned that even though a good understanding of these materials was gathered through detailed structural characterization, the performance characteristics of these materials were not quite appealing yet.

Reviewer 3:

The reviewer confirmed that the results certainly helped the research community to understand the limitations/opportunities with these compounds. The reviewer suggested that using mAh/g might not be the best metric to report the capacity of these compounds since the voltages are around 2 V or below, thus reporting a 200 mAh/g capacity does not tell the true story.

Reviewer 4:

The reviewer asserted that the insertion of Li into LiVOPO₄ has caused a significant potential reduction to the level that it becomes not practically useful. The reviewer recommended that the electrical conductivity of synthesized LiVOPO₄ should be measured.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer affirmed that a number of key, and well-known, laboratories were involved in the consortium.

Reviewer 2:

The reviewer simply noted that Dr. Manthran was always willing and able to assist.

Reviewer 3:

The reviewer said that there is no formal collaboration yet for this project. Though exploratory in nature, some collaboration with a national laboratory or industry in terms of assessing the performance of the cathode materials will help in prioritizing these materials and focusing on the promising candidates for further development.

Reviewer 4:

The reviewer noted collaboration with Lawrence Berkeley National Laboratory (LBNL) on x-ray absorption and Oak Ridge National Laboratory (ORNL) on XRD has been developed.

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.**Reviewer 1:**

The reviewer offered that the future work is focused well to advance the battery research community's understanding of these classes of cathode materials. The reviewer was curious to see how nanoparticles affect the capacity as well as how the proposed dopants modulate the cell voltages.

Reviewer 2:

The reviewer remarked that the future work on the use of graphene as a conductive diluent was very interesting and a promising method for maintaining contact to the particles of active materials.

Reviewer 3:

The reviewer explained that the proposed future research is to continue the development and study of the three polymorphs of LiVOPO_4 cathode and to downselect one for further study on the synthesis of LiVOPO_4 /graphene nanocomposites to improve conductivity and thus increase the capacity to approximately 250 mAh/g. Likewise, the aliovalent doping of M (in LiMPO_4 ; M=Fe, Mn, or Co) as well as Li_2MSiO_4 and $\text{Li}_2\text{MP}_2\text{O}_7$ (M = Mn, Fe, Co, and Ni) with V^{3+} or Ti^{4+} will be explored to improve their ionic and electronic conductivities. The reviewer reinforced that the proposed materials look interesting, but this person noted that the approach seems to be truly exploratory and non-specific. The expected improvements did not appear to be significant to the reviewer compared to some of the known layered mixed metal oxide materials (Ni-rich or LMR-LLC). The reviewer suggested that the materials need to be prioritized, or ruled out, based on their performance to make this effort beneficial to the DOE Applied Battery Research for Transportation program.

Reviewer 4:

The reviewer suggested that the PI should investigate how to improve the cyclability and charge/discharge rate of LiVOPO_4 . The reviewer also requested that the PI should also make an extensive literature search for previous works on the doping of LiFePO_4 and LiMnPO_4 .

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer explained that low specific energies and high costs of Li-ion batteries are serious impediments to their widespread adoption in vehicles. Thus, improvements in the specific energy of electrode materials will result in increased range for the vehicle as well as reduced overall cost for the battery. The reviewer stated that state-of-the-art cathode materials have low capacities due to their inability to intercalate with more than one Li ion per transition metal. The reviewer proposed that the researcher community needed to explore new cathode materials that can intercalate multiple Li-ions and or provide higher capacity than the state-of-the-art materials, which the present project is duly addressing.

Reviewer 2:

The reviewer agreed that a high capacity, stable cathode was critical for developing an efficient, low-cost battery.

Reviewer 3:

The reviewer affirmed that the work directly supported the DOE VTO program and provided a new look/method for improving contact between the cathode materials and the current collector.

Reviewer 4:

The reviewer stated that the project was developing a high capacity high-voltage cathode for Li-ion batteries.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer simply stated that the support was adequate.

Reviewer 2:

The reviewer agreed that the resources were adequate for the scope of the project.

Design of High Performance, High Energy Cathode Materials: Marca Doeff (Lawrence Berkeley National Laboratory) - es052

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that the approach is in keeping with the traditional method for developing new cathode materials for Li-ion cells. The reviewer complimented that the PI is a careful worker and a fountain of knowledge of the past work at LBL.

Reviewer 2:

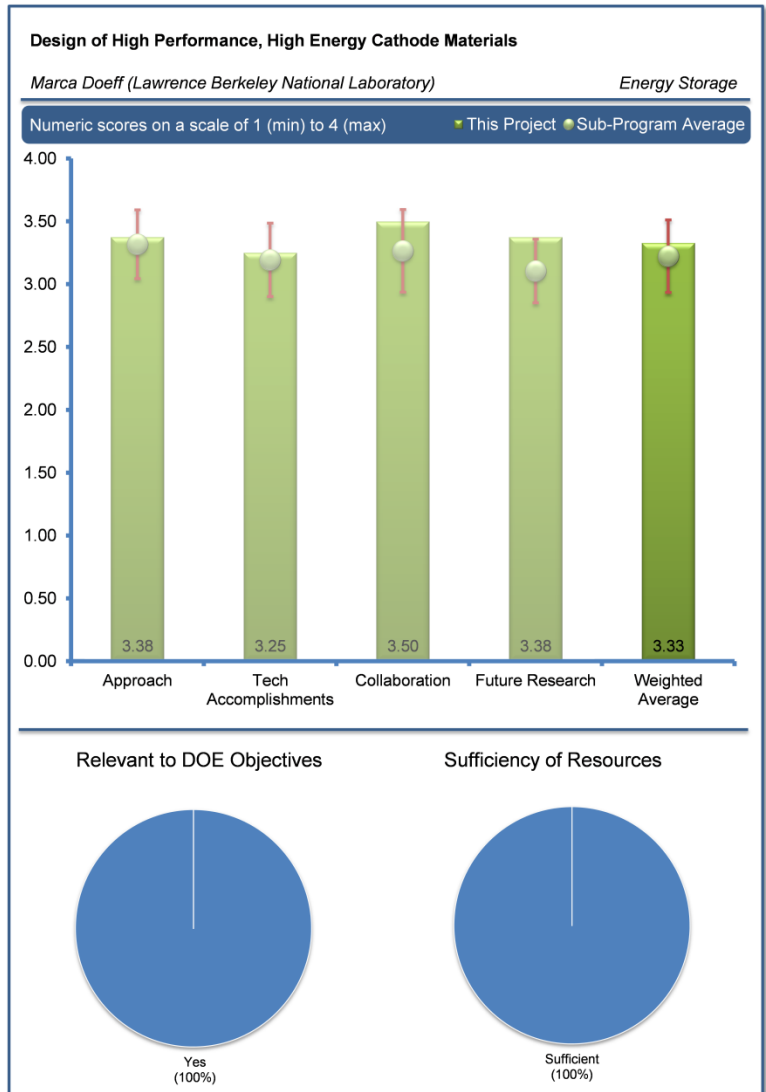
The reviewer affirmed that soft XAS and HRTEM have been effectively used to study the surface properties of aging cathodes.

Reviewer 3:

The reviewer explained that the project objective is to develop high-energy cathode materials with layered composites, with particular emphasis on modified NMCs, and to optimize their synthesis using a low-cost spray pyrolysis method. The reviewer noted that the spray pyrolysis method is a one-step process yielding the desired morphology, and also allows simultaneous doping and subsequent surface coating. The reviewer indicated that although titanium substitution into NMC is not new, its substitution for Co^{3+} here (instead of Mn^{4+}) is mainly responsible for the improved performance. Detailed analytical studies, using soft X-ray absorption spectroscopy (XAS) and other synchrotron techniques are being carried out to understand the mechanism underlying the improvements from titanium (Ti)-doping. The project person agreed that the approach overall is effective, and that the spray-pyrolysis method is proving to be feasible for the development new cathode materials. However, the reviewer noted that the cycle life data shown with the Ti-doped MNC materials, though better than the pristine materials at higher voltages, is not promising with rapid capacity fade within 20-30 cycles. The reviewer commented that proper trades are to be made to establish the merit of these materials in comparison to the other mature options (e.g., conventional coated cathodes).

Reviewer 4:

The reviewer remembered seeing people make attempts to use spray pyrolysis for spinel synthesis a long time ago. The reason was forgotten, but this reviewer recalled that it never caught on and the large difference in melting/decomposition the authors refer to might further complicate the scenario. The reviewer cautioned that even the data are not too supportive that this will be a right approach to solve the life issues. The reviewer also suggested that such a process might not be the one that is commercially-attractive.



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.

Reviewer 1:

The reviewer stated that good progress had been made and the project goals were met.

Reviewer 2:

The reviewer remarked that the diagnostic data are quite impressive. The reviewer thought that the authors were capable of doing a much better job in that regard, than on the synthesis/processing part.

Reviewer 3:

The reviewer explained that impressive fundamental analytical studies were carried out to understand the capacity degradation in NMC cathodes during cycling at high voltages. It was shown that the NMC particles are covered with a rock salt layer comprised of reduced Ni, Co, and Mn, which may be primarily responsible for the capacity loss. The reviewer reported that Ti-substitution is speculated to be modifying the composition of this surface layer to make it more conductive (perhaps being inferred from electrochemical impedance spectroscopy). The reviewer suggested that spray pyrolysis appeared to be a simpler and lower-cost method compared to the standard co-precipitation/calcination, but the (hollow) morphology is not optimum for high tap densities. Even though the cyclic stability is improved with Ti compared to pristine materials, the cycle life data with Ti-doped NMC is not impressive yet, with rapid capacity fade within 20 cycles. The reviewer summarized that even though a good understanding of these materials was gathered through detailed structural characterization (which resulted in good publications), the performance characteristics of the Ti-doped NMC materials are not quite appealing yet.

Reviewer 4:

The reviewer commented that the project has been focused on the surface reconstruction and valance change of surface element. The reviewer stated that HRTEM with SAED can be used to study the microstructural and crystalline change inside the aging cathode particles.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer confirmed that the collaboration with other institutions and the work program was coordinated with others in the DOE network.

Reviewer 2:

The reviewer commented that there were useful collaborations within LBNL and with external laboratories to carry out the soft XAS and other synchrotron studies.

Reviewer 3:

The reviewer recognized that the PI has established a wide collaboration with several institutions including the Stanford Synchrotron Radiation Lightsource for XAS, Brookhaven National Laboratory (BNL) for transmission electron microscope, and the University of California, Berkeley for computer modeling.

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.

Reviewer 1:

The reviewer stated that the proposed work is in keeping with the program goals and should make significant contributions.

Reviewer 2:

The reviewer described that the proposed future research is to continue the study of the rock salt formation in the NMC cathodes, using additional synchrotron, X-ray Raman measurements. The spray pyrolysis/infiltration method will be extended to other classes of cathodes such as $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$, $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$, and NMCs with higher Ni content. Further, the reviewer explained that these cathodes will be coated with surface coatings for stability at high charge voltages, with the coatings powders (Al_2O_3 , ZnO) made by spray pyrolysis. The reviewer explained that even though the long-term cyclic stability of Ti-doped NMC is questionable (or not demonstrated yet), the spray pyrolysis method is promising and merits further study with other potential cathode materials.

Reviewer 3:

The reviewer noted that X-ray Raman will be introduced to provide additional information about surface structure; however, the crystallinity and composition change inside bulk should also be studied.

Reviewer 4:

The reviewer observed that the project team's experience tells us that work related to coatings using ZnO and Al_2O_3 will be waste of time since it is not effective in the long run.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer agreed that the availability of high-performance battery systems will speed the development of electric propulsion for all levels of automobiles.

Reviewer 2:

The reviewer affirmed that the low specific energies and high costs of Li-ion batteries are serious impediments to their widespread adoption in electric vehicles. High energy density electrode materials will result in improved specific energy for Li-ion cells, increased range for the vehicle, as well as reduced overall cost for the battery. The reviewer stated that the state-of-the-art cathode materials provide capacities of only approximately 160 mAh/g, or about half of the capacities from the carbon anodes. The reviewer confirmed that the battery research community needs to explore new cathode materials with higher specific capacity and voltage, while maintaining the stable layered structures of the cathodes, which the present project is addressing.

Reviewer 3:

The reviewer agreed that understanding of surface properties will provide useful information for improving cathode capacity and cyclability.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that sufficient resources are available.

Reviewer 2:

The reviewer commented that the resources are adequate for the scope of the project, but cautioned that it may be a little on the high side.

Reviewer 3:

The reviewer asserted that it appeared that LBNL has a very high overhead.

First Principles Calculations of Existing and Novel Electrode Materials: Gerbrand Ceder (Massachusetts Institute of Technology) - es054

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

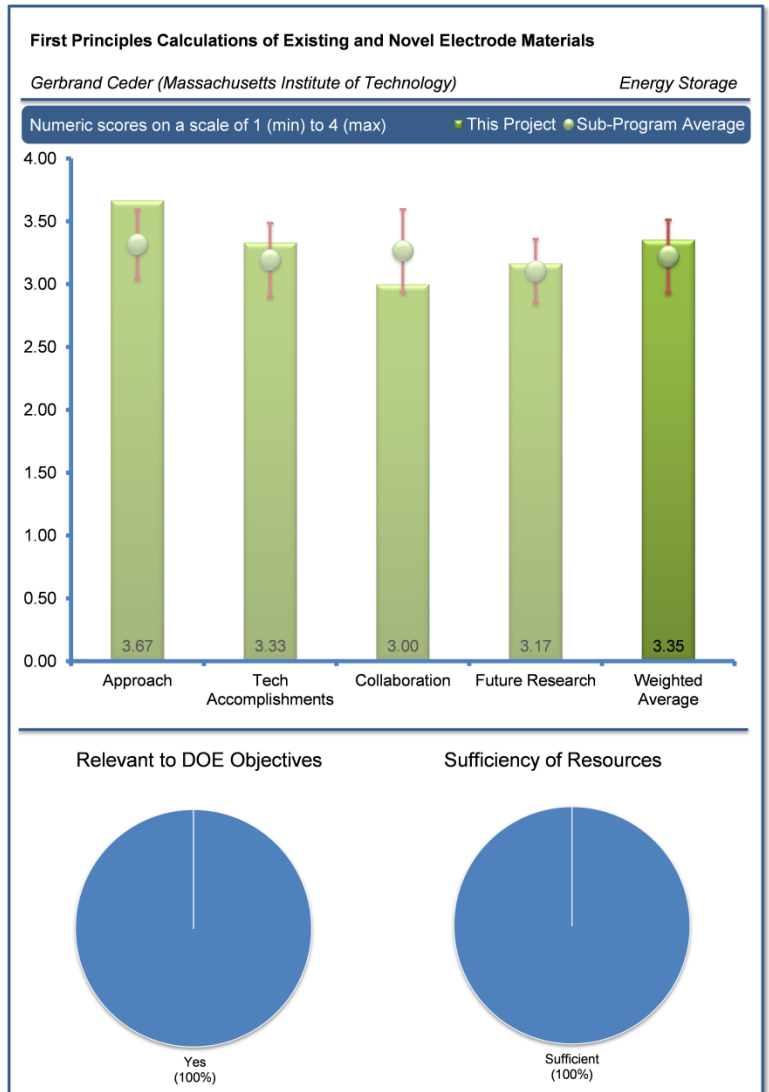
The reviewer recognized that the PI's use of several complementing theoretical tools to examine the stability, transport, and voltage of many electrode active materials is very useful. The reviewer acknowledged that seeking out fundamental mechanisms and new high capacity positive electrode materials is a huge challenge that the PI has readily taken on these activities. The reviewer pointed out that there is a lot of interest in sodium-ion materials, that the reviewer was not sure was justified. Nevertheless, this reviewer said it will be interesting to see the PI's results on this aspect of the project.

Reviewer 2:

The reviewer commented that the mapping of the potential energy for Li-ion diffusion path reminded them of a text book, which density functional theory studies should be. The reviewer asked whether it would be possible to see a comparison of the calculated diffusivity and the experimental data. The reviewer suggested that the computation for the bulk structure may not represent exactly the electrochemical behavior since the electrochemistry is often controlled by the surface structure of the material which is not exactly an extension of the bulk structure. Namely it is highly possible that the lattice parameter and/or the oxidation state of the electrode particles near the surface are different from those of the bulk material.

Reviewer 3:

The reviewer affirmed that this is an important contribution that is trying to explain Li mobility on relation to the state of charge of the material. The reviewer pointed out that the presenter stated that "in layered materials slab spacing contracts at low Li concentration, thereby reducing Li mobility, and reducing practical charge capacity." It seemed to this reviewer that Li is also shielding the negative charges from the oxygen atoms above and below the Li layer. The reviewer asked if it can also be said that as Li is removed, the Li that remains in that layer is more tightly bound to the oxygen atoms. The reviewer also stated that, in the areas where Li has been removed, the oxygen-oxygen repulsion should increase, so asked whether that would result in a less noticeable contraction of the slabs.



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.**Reviewer 1:**

The reviewer commented that, as done by the author, a correlation of experimental information with theoretical calculations is very valuable. The reviewer hoped that the author continued in this direction. The reviewer proposed that additional insight and guidance could be provided to the experimentalist for the design of better cathode materials.

Reviewer 2:

The reviewer stated that it would provide a better solid ground for the approach if more extended experimental data including cycling performance were shown.

Reviewer 3:

The reviewer praised that the PI is very productive in several areas. In the work on highly-lithiated materials, it was not clear to the reviewer whether the PI considers the case of the material being a composite structure and how that would influence the results. The reviewer also highlighted that the PI's work with MoCr transition metal oxides is interesting, but it is not clear to this person how these materials will ever get into a transportation application. It was also not clear to the reviewer how many different materials were studied by the PI. The reviewer would like to see the PI try to verify the results with experimentation.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer acknowledged that it was good to see collaboration with experimentalists.

Reviewer 2:

The reviewer commented that the program is fairly new, so thought that additional collaborations will probably be seen in the future.

Reviewer 3:

The reviewer remarked that the PI lists only a limited number of collaborations.

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.**Reviewer 1:**

The reviewer commented that, as suggested by the author, further connection with the Li-excess ANL-style materials should be strongly pursued.

Reviewer 2:

The reviewer asked how useful the sodium-ion material is. This person also asked what the projected anode material was and how practical the chemistry was.

Reviewer 3:

The reviewer expressed not being overly excited by the proposed future work that based on the PI's present efforts. The reviewer acknowledged that the PI will continue to study the MoCr system, rather than looking for other more relevant materials. The reviewer acknowledged that the PI's interest in highly-lithiated materials is more than justified, but did not indicate that more complex structures will be considered.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer acknowledged that the PI made a solid case for relevance. The reviewer, however, was not sure how general one can be, but liked the plot with material capacity using different anions.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer stated that the PI seems to have sufficient resources to attack the difficult problems on multiple fronts.

First Principles Calculations and NMR Spectroscopy of Electrode Materials: Clare Grey (University of Cambridge) - es055

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer claimed that the PI is in the unique position that brings the in-situ nuclear magnetic resonance (NMR) techniques for better understanding the battery material behavior that often is difficult to characterize by other techniques. The reviewer wondered if the PI could look at other state-of-the-art materials instead of the high-voltage spinel that has been well-studied by in-situ synchrotron X-ray probes in the literature.

Reviewer 2:

The reviewer emphasized that this was world-class work in the methodology of multi-NMR. The reviewer remarked that it was important for the researcher to keep in close contact with the battery community to be sure to be working on the most important problems to batteries. The reviewer explained that the technique was unique in revealing the details of the environment around the nucleus under study and that we are fortunate that Li has an isotope with reasonable abundance that has a nuclear magnetic moment that is available for study.

Reviewer 3:

The reviewer reported that NMR studies on these advanced electrode materials give the battery research community a unique chemical insight into their operation and degradation mechanisms. Further, the PI's focus on silicon materials is also pertinent. Finally, the reviewer asserted that the use of in-situ studies is very good.

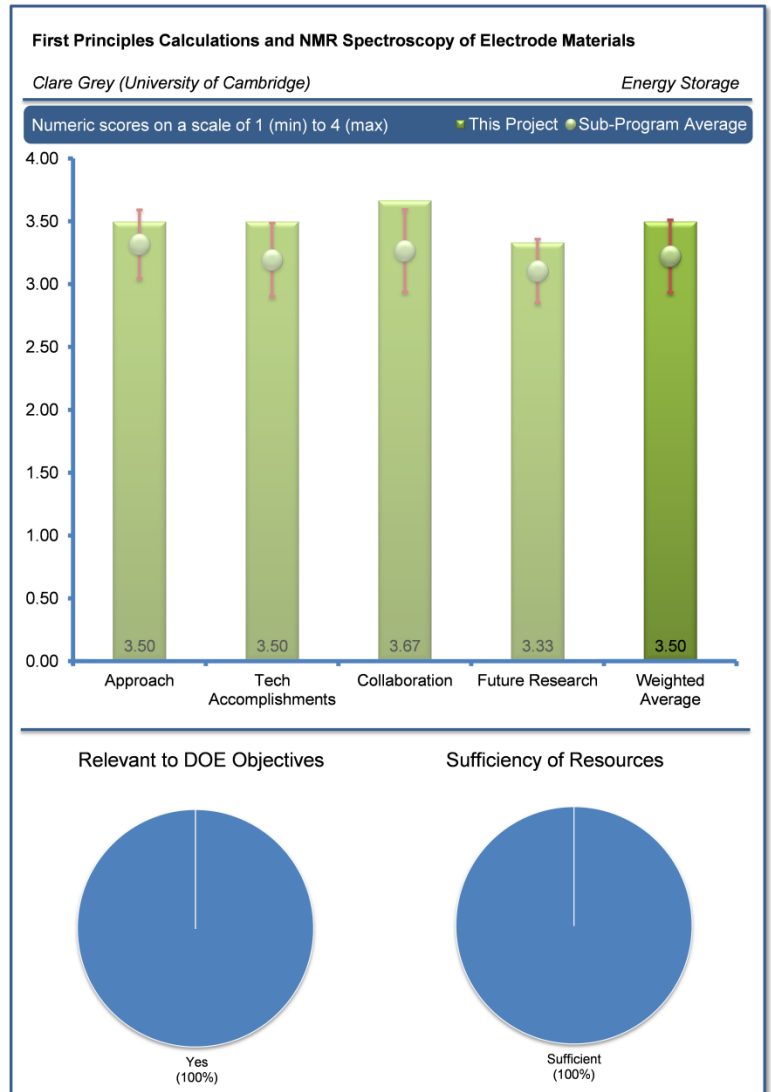
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer recognized that the NMR studies of solid electrolyte interphase (SEI) layers in collaboration with the electrolyte/additive specialist are good.

Reviewer 2:

The reviewer recounted that the work on Si lithiation has been very revealing of the mechanism for lithiation as a function of Li level. This person noted that the information developed on the SEI formation on lithiated silicon will be quite valuable in helping to design a high-energy silicon electrode with good cycling capability. The reviewer also explained that the work on high-voltage spinel is also



revealing for determining the differences between the ordered and disordered forms of the material and the reflection on electrochemical performance differences. The reviewer mentioned that the work on tortuosity is novel and will be useful to electrode designers if the results are translated to the field.

Reviewer 3:

The reviewer explained that the PI chiefly utilizes NMR integrated with electrochemical and other diagnostic techniques, which adds a unique perspective on battery studies. Further, the PI has conducted a wide array of studies on a number of pertinent electrode materials. The reviewer recognized that the PI's focus on the Si and its SEI is very timely.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer commented that the PI is known to have an extensive collaboration network that involves the best battery material scientists.

Reviewer 2:

The reviewer expressed that most of the collaborations are long-standing and well-developed. The reviewer suggested that it would be good to include some collaborators in the tortuosity field to highlight important problems in this field as well.

Reviewer 3:

The reviewer stated that the PI has an extensive list of collaborations.

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.**Reviewer 1:**

The reviewer simply remarked that the outstanding work was expected to continue.

Reviewer 2:

The reviewer indicated that the PI's future work is an extension of their present work.

Reviewer 3:

The reviewer asked whether the PI had any interest in ANL's materials or coating materials.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer agreed that the work on Si and high-voltage cathodes and on diffusivity/tortuosity measurements is highly-relevant to battery issues.

Reviewer 2:

The reviewer praised that the PI is carrying out very relevant work, although the reviewer did not think the PI necessarily has made the best case for the importance of their work. The reviewer also noted that the relevance slide seems to have been an afterthought at the bottom of the overview slide.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer said that, based on the PI's productivity, the project seems to have sufficient resources.

Development of High Energy Cathode Materials: Jason Zhang (Pacific Northwest National Laboratory) - es056

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer described that Dr. Zhang's work has concentrated on the synthesis of lithium-manganese rich (LMR) layered composite cathode materials as a means to identify cost-effective approach to their commercial production. In particular, the PI has used advanced instrumental approach to better understand the failure mechanisms of the LMR cathode materials and develop electrolyte additives to improve the stability for long cycle life.

Reviewer 2:

The reviewer explained that the project objective is to understand the mechanisms contributing to the capacity loss of the LMR-LLC cathode materials and to improve their cycle life by modifying the electrolyte formulation, elemental doping of the cathode, and developing alternate low cost hydrothermal assisted synthesis of these cathode materials. The reviewer agreed that this project thus addresses one of

the key performance barriers of the LMR-LLC cathodes, and adopts a viable approach and is well-integrated with the other efforts in understanding/mitigating the voltage fade. The reviewer expressed that it would be better to have this project coordinated through ANL for better synergy, based on the substantial effort being undertaken at ANL on various aspects of the LMR-LLC cathodes.

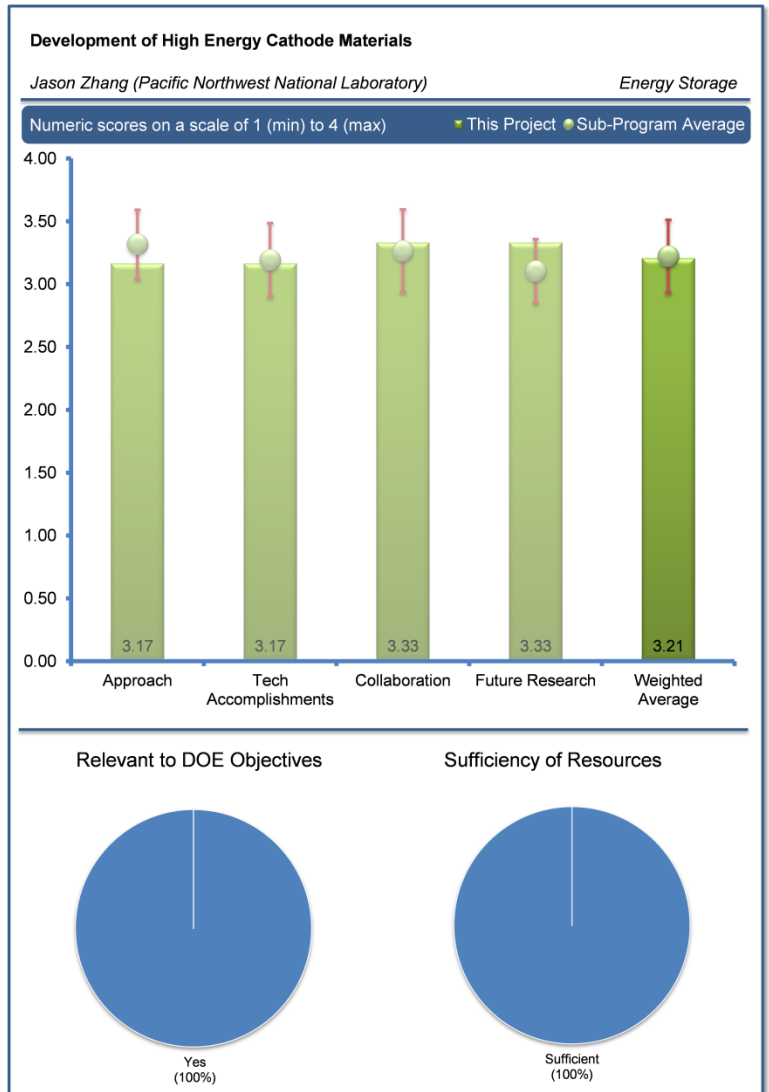
Reviewer 3:

The reviewer observed that the data indicates that synthesis routes or use of additives, although appearing beneficial to some degree, are some temporary measures to retard the eventual evolution of voltage decay or poor cycle-life.

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.

Reviewer 1:

The reviewer asserted that the improvements were good, but this person was not sure they will hold at elevated temperatures or in the course of long-term cycling. The project person praised that the analytical work the authors have carried out to identify the failure mechanism was quite good.



Reviewer 2:

The reviewer indicated that good progress has been made in understanding the performance fade of the LMR-LLC cathodes from the elemental distribution and the Ni segregation. The reviewer summarized that the cathode particles tend to fragment due to the stresses originating from the oxygen release, which in turn change the Mn valence from the bulk. The hydrothermal-assisted synthesis appears to reduce the problem of Ni segregation on the surface as well as the voltage fade to some extent. The reviewer also noted that the cycle life is also improved with this synthetic approach. The reviewer requested that the cathode loadings adopted here should be included (example on Slide 9). The reviewer noted that the LMR-LLC cycle life looks impressive, but only at low loadings. The reviewer also indicated that the cycle life improvements with the additive TFPB (though not new), attributed to reduced SEI and the increased oxygen solubility, are encouraging. The reviewer pointed out that there were some good publications that emerged from this project. The reviewer reiterated an earlier comment that this project needed to be aligned with the ANL effort on the LMR-LLC cathodes.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer recognized that there were good collaborations with the other DOE laboratories and external university partners.

Reviewer 2:

The reviewer pointed out that Dr. Zhang followed the work at other institutions as well as the publications in the current literature, and as a result was a good source of information of the work in this field.

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.**Reviewer 1:**

The reviewer stated that the proposed work appeared to be quite extensive and well thought out. The reviewer proposed that modulating the Ni/Mn ratio or the use of additional dopants might be an effective route to fundamentally improve the LMR stability.

Reviewer 2:

The reviewer stated that the proposed work is in keeping with the need for improved performance from cathode materials.

Reviewer 3:

The reviewer described that the proposed future research is to continue improving the hydrothermal-assisted synthesis methodology with the objective of identifying the key parameters for layered-to-spinel phase transition, for example by optimizing the Ni/Mn ratio in LMR to balance the specific energy and cyclic stability. The reviewer reported that it was observed that the voltage fade appeared to be a minor component of the energy fade upon cycling, which the reviewer tends to agree with; the capacity fade is as serious a problem if not more. The goal remains to be a better understanding of the changes in the interfacial and bulk properties of the LMR-LLC cathodes during cycling. The reviewer concluded by stating that the future plans were consistent with overall goals of the DOE Applied Battery Research for Transportation program.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer emphasized that the low specific energies and high costs of Li-ion batteries are serious impediments to their widespread adoption in vehicles. LMR-LLC cathode materials are promising both from an energy and cost perspective, but are hampered by issues such as capacity and voltage faded upon cycling. The reviewer affirmed that it is essential to improve the cycle life of these high-energy materials to make them applicable for EV applications, as is being done in the present project.

Reviewer 2:

The reviewer expressed that, because of its very large capacity and potential low cost, work on LMR will go a long way in developing a long-life, low-cost battery.

Reviewer 3:

The reviewer indicated that the successful conclusion of Dr. Zhang's work will add significantly to the available knowledge of cathode materials and provide more options in selecting commercial electrode materials.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer commented that the resources were reasonable and available for the success of the project.

Reviewer 2:

The reviewer stated that the resources were adequate for the scope of the project.

Advanced in-situ Diagnostic Techniques for Battery Materials: Xiao-Qing Yang (Brookhaven National Laboratory) - es059

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer agreed that monitoring oxygen generation during charging and discharging the cathode materials is an excellent approach to identify the operation voltage range for the given materials. The reviewer also commented that in-situ XRD and XAS are powerful tools for understating the battery chemistry that potentially address the issues the battery research community faces.

Reviewer 2:

The reviewer explained that the use of high- and low-energy X-ray beams at the BNL facility has proved to be very useful in determining structures of active materials at various stages of charge and discharge as well as time resolved studies which have been useful in determining kinetic factors is electrode reactions. The reviewer reported that the approach has been well-validated by the researcher and coworkers. The reviewer also pointed out that unique studies have been carried out by combining X-ray absorption studies in parallel with diffraction studies to advance the state-of-the-art. The project person recognized that the author has been able to develop important collaborations to ensure that key problems of interest to the DOE VTO program have been attacked. The reviewer reported that the closing of the BNL National Synchrotron Light Source will necessitate a revision of the work scheduling until the new light source is available; Dr. Yang is developing such plans according to a follow-up discussion.

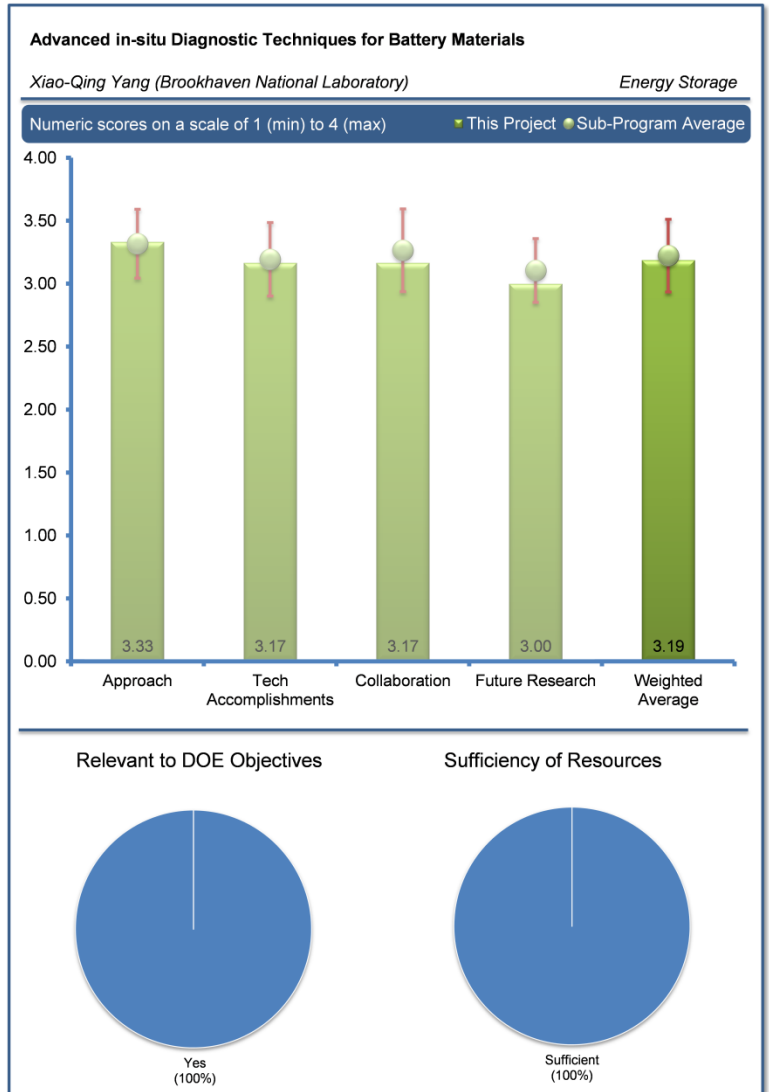
Reviewer 3:

The reviewer commented that the PI has been studying pertinent electrode materials using mainly XRD and XAS, combined with electrochemical and thermal studies, for many years. The reviewer highlighted that the PI continuously works to expand the toolset used to examine these materials. The approach this year represents another solid year of studies.

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.

Reviewer 1:

The reviewer indicated that it can be better if full analyses of Extended X-Ray Absorption Fine Structure data are carried out. The reviewer also mentioned that this group has an excellent track record.



Reviewer 2:

The reviewer reported that the accomplishments have been excellent and have revealed interesting facts concerning the operation of Li excess materials, high-voltage spinel materials (including the important differences in properties of ordered and disordered materials).

Reviewer 3:

The reviewer claimed that this work seems to be similar to other XRD and XAS work being conducted under this program and elsewhere. The PI's extensive use of in-situ studies and mass spectrometry to detect released gasses are two aspects of this work that help make it special. The reviewer also mentioned that the PI's past experience with battery materials is another plus. The reviewer particularly liked the PI's discussion of the proposed mechanisms.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer stated that this group has a good research network.

Reviewer 2:

The reviewer indicated that the researcher has fostered a number of long-term collaborators to keep up with the important battery problems. The reviewer noted that the PI recognizes that the collaborations need to expand the collaborations with U.S. industry and academic researchers, however and the reviewer agrees with this effort for the future.

Reviewer 3:

The reviewer said that the PI has collaborated extensively with several institutions around the world.

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.**Reviewer 1:**

The reviewer simply stated that the PI proposed to continue the present studies.

Reviewer 2:

The reviewer wondered if the studies of voltage fade on the ANL material by in-situ XRD and XAS were organized with the ANL group (e.g., Croy's team).

Reviewer 3:

The reviewer explained that there were some uncertainties about future projects because of the closing of the light source. The reviewer pointed out that for some time it will be necessary for the group to travel to other synchrotrons in order to accomplish new studies; this will require considerably more planning. The reviewer also noted that the development of new collaborators will require careful thought to optimize the collaborative results.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer agreed that the work had good relevance to DOE objectives.

Reviewer 2:

The reviewer confirmed that these studies were very relevant, although the PI did not make a very good argument.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that the sooner the new light source was available, the better the resources were for the kinds of studies to be carried out by this project.

Reviewer 2:

The reviewer remarked that based on the PI's productivity, the resources were adequate.

Nanoscale Heterostructures and Thermoplastic Resin Binders: Novel Li-ion Anode Systems: Prashant Kumta (University of Pittsburgh) - es061

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer simply stated that the approach is good and meaningful.

Reviewer 2:

The reviewer agreed that the technical approach was interesting, but suggested that the cost for h-SiNT may be a barrier for the potential commercialization of the material.

Reviewer 3:

The reviewer commented that the work presented targeted the specific objectives regarding improvement of the anode active material, and addresses the issues of the anode-binder-electrode structure interfaces.

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.

Reviewer 1:

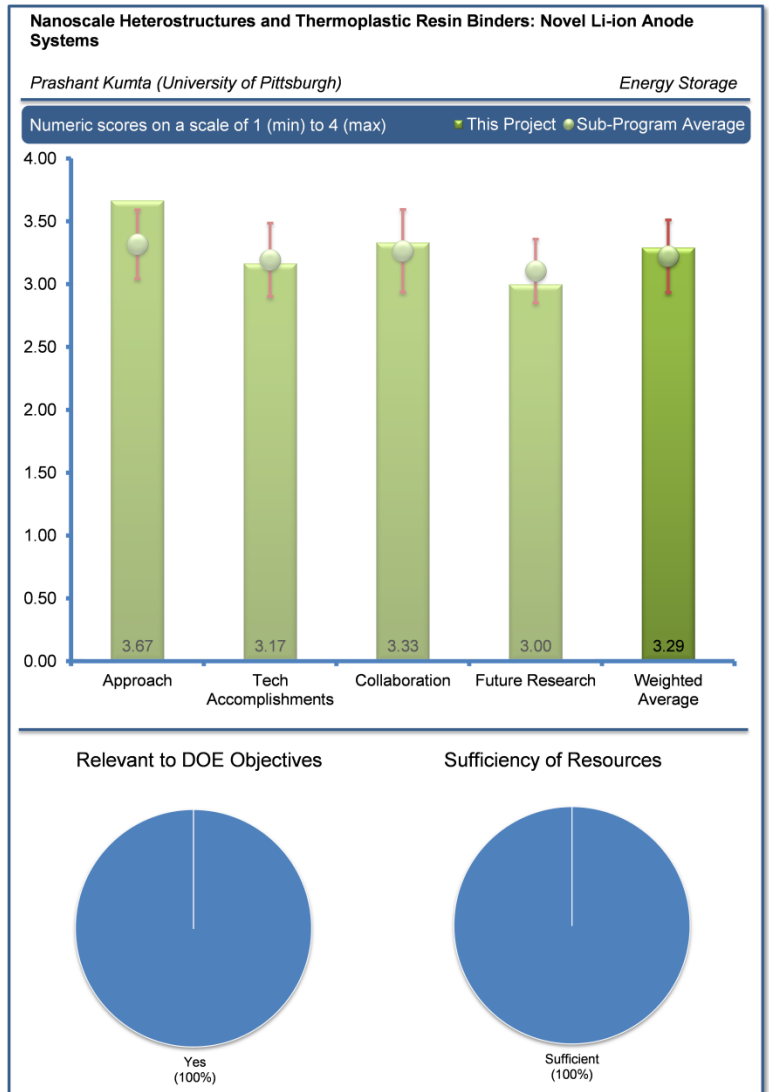
The reviewer reported that several types of Si, and or their composites, have been studied and the results are promising. However, the reviewer cautioned that some challenges remained such as the charge/discharge efficiency was still relatively low and the capacity decay was still high. The reviewer suggested investigating and understanding the correlation of the charge/discharge efficiency. Hopefully that will help to explain the correlation of the efficiency and the materials structure.

Reviewer 2:

The reviewer explained that the investigator selected two differing approaches to address the active material structure. The issue the reviewer had was that a clearer demonstration of the gaps against the DOE performance and cost objectives as a function of project progress would be beneficial.

Reviewer 3:

The reviewer described that h-SiNTs were tested at very high current rates (10 A/g) and showed a decrease in capacity in the beginning cycles compared to the other capacity measurements performed at (2 A/g) that showed an increase in capacity for up to 50 cycles and then decrease to a steady state. The reviewer asked how the loading in the electrodeposited films could be improved. This person also



asked if any post-mortem analysis of high strength binder, especially PE and composite binders, had been done. The reviewer observed that the broad resonances in the region 3.0-4.2 ppm corresponding to the polypropylene polymer seemed to be shifted and enhanced after cycling.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that the collaboration was solid.

Reviewer 2:

The reviewer indicated that the collaboration had been improved.

Reviewer 3:

The reviewer suggested that it would have been helpful if the slides for reviewers to review had one or several bullet points talking about the contribution of the collaborators to this project. For example, the reviewer asked what Ford Motor Company's contribution was and how the company was involved in this project.

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.

Reviewer 1:

The reviewer reported that several approaches had been proposed for the future work. The reviewer hoped a Go/No-Go plan with targets could be listed. The proposed coating approach may not solve the FIR decay problem completely if the broken electric contacts are the major issue. The reviewer asked whether it was possible to try any conductive binders in this project.

Reviewer 2:

The reviewer stated that the approach to future work was general. The reviewer described that the two approaches used for active material design led to two difference electrode designs, and with differing problems to be resolved. The PI should clarify which improvements applied to which method.

Reviewer 3:

The reviewer explained that the future research included improving the areal capacity of electrodeposited Si film by using stacked multilayered composite electrode of [a-Si/C]/n. The reviewer suggested that adhesion of the films should be considered. The reviewer also suggested that the researchers considered improving the electronic conductivity of the binder.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer explained that the objective of this study was to investigate Si anodes as a potential graphite anode replacement for increased battery energy density.

Reviewer 2:

The reviewer praised that the project was a solid example of innovation; success in this area would support the delivery of higher energy density cells.

Reviewer 3:

The reviewer commented that the project reduced the consumption of fossil fuel resources and pollution.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer said that it appeared the researcher had sufficient resources and collaborators to conduct the proposed research.

Reviewer 2:

The reviewer noted that the overall program management was sound, and that the resources appeared to have been managed appropriately.

Reviewer 3:

The reviewer reported that the resources were sufficient for the project.

Metal-based High Capacity Li-ion Anodes: Stanley Whittingham (Binghamton University, State University of New York) - es063

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer commented that the work addressed a critical barrier to increase anode volumetric capacity and gravimetric capacity as well as the anode.

Reviewer 2:

The reviewer described that the applied technical approach demonstrated a good example of multivariate design approach. The reviewer was interested to see the PI's recommendation for the most promising of all routes employed.

Reviewer 3:

The reviewer observed a good approach, and inquired about how good the Sn-Fe-C composite is compared to Sn-Co-C.

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.

Reviewer 1:

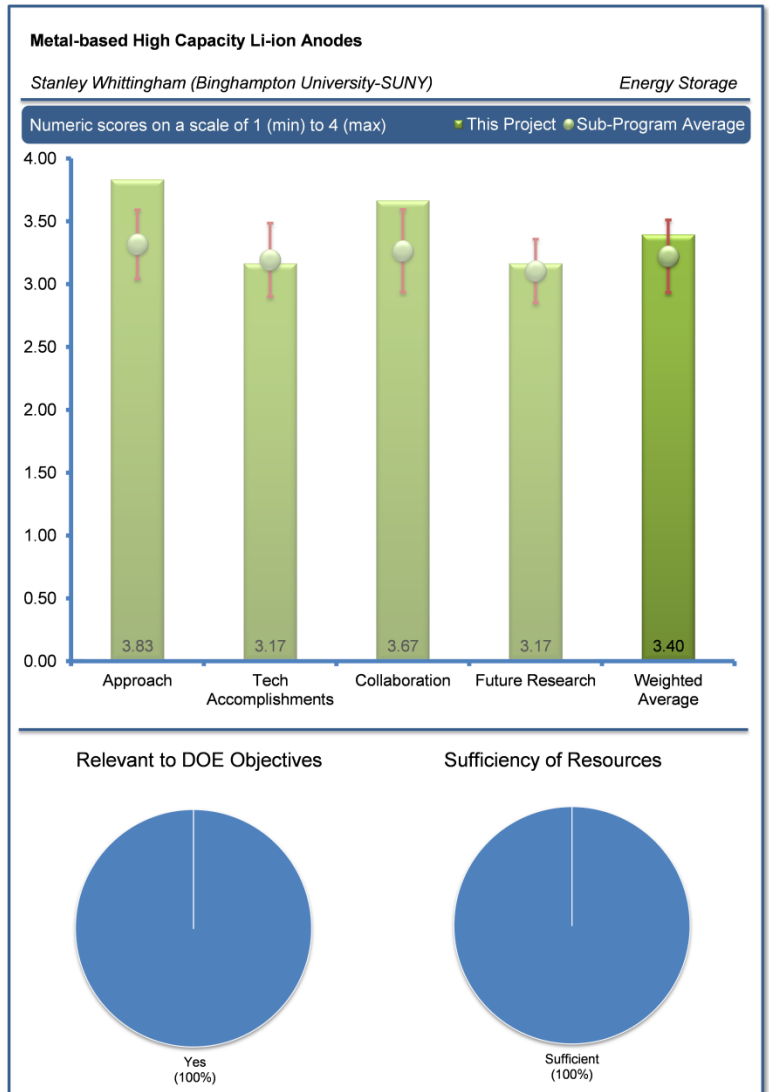
The reviewer praised that this project has so far achieved goals that surpass the original goals; for example, 2.0 Ah/cc had been achieved when compared to 1.6 Ah/cc of original goal. It was unclear to the reviewer what the volumetric capacity and gravimetric capacity were at a higher rate.

Reviewer 2:

The reviewer observed that the results of the work address energy density (specific capacity), cyclability, and general stability, but that calendar life and cost have yet to be addressed. This person also stated that it would also be beneficial to see the supporting calculation for the claim to a potential 50% improvement in cell energy density.

Reviewer 3:

The reviewer indicated that a comparison slide for all the methods with capacity would be helpful, instead of switching back and forth between volumetric capacity and specific capacity for tin (Sn), Sn-Fe, Sn-Fe-C composite. In the methods of mechanochemical synthesized Sn-Fe-C and solvothermal synthesis of Sn-Fe composite, the reviewer asked how much carbon is involved and how does the carbon content affect similar to tin in Slide 11. The reviewer also asked what the reason is for the better capacity when Sn-Fe composite ratio is 5:1.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer said that this project has a strong collaboration with other institutions.

Reviewer 2:

The reviewer reported no issues.

Reviewer 3:

The reviewer indicated that the collaboration was good.

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.**Reviewer 1:**

The reviewer suggested adding the cycling performance versus rate in the go/no-go targets.

Reviewer 2:

The reviewer suggested that the PI investigate more closely the cost-related claims (with support from an external resource, potentially a battery maker), as well as the technical viability for material scale-up (paper study, not demonstration).

Reviewer 3:

The reviewer explained that graphite converts to active carbon reacting to give LiC_2 was mentioned; this might enhance the SEI layer formation similar to carbon. In addition to determining the impact of carbon-type, the reviewer suggested that the amount of carbon used should also be considered.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer stated that the work addressed battery energy density and specific energy improvement by addressing critical barriers to improve anode volumetric capacity and gravimetric capacity.

Reviewer 2:

The reviewer commented that this anode work had good potential in improvement of cell energy density and safety, and potentially cost.

Reviewer 3:

The reviewer agreed that the project targets reduced petroleum use and emissions.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that there were sufficient resources allocated for this project.

Reviewer 2:

The reviewer reported that the good management of resources, as well as program management. No issues in the management of the project were observed.

Reviewer 3:

The reviewer said that sufficient resources were available for the project.

Development of Electrolytes for Lithium-ion Batteries: Brett Lucht (University of Rhode Island) - es067

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer asserted that the investigator was one of only a few researchers in the electrolyte field and continued the high performance and excellent science applied to battery related materials. The reviewer confirmed that new stable electrolytes were essential for continued development of high-performance electrode materials; adding that the work has concentrated on electrolytes for cells with high-performance silicon anodes. The reviewer explained that the approach was to use ex-situ surface analysis to understand the interaction of the anodes with the electrolyte and develop an understanding of the using FEC and VC. The reviewer said that the initial results are very promising.

Reviewer 2:

The reviewer expressed that the refocus on the SEI was important. The reviewer also noted that the technical barriers were addressed properly.

Reviewer 3:

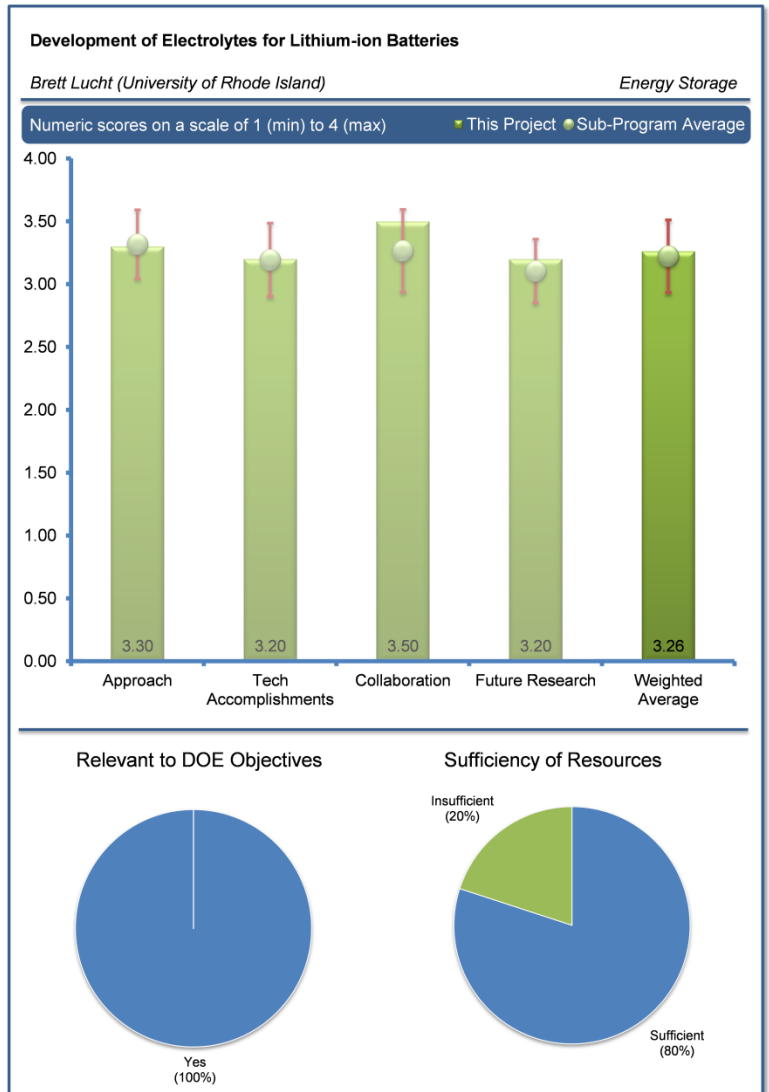
The reviewer applauded that the team has done an excellent job on the initial screening of the effects of different additives on SEI formation on Si anodes in a very short period of time. The reviewer recognized that the team understands that the systematic approach is necessary to optimize the composition. The reviewer commended that the team is using different thicknesses Si electrodes to study effects of electrolyte formulations; this is very important to continue and provide reasons for the difference in performance.

Reviewer 4:

The reviewer asserted that a well thought-out approach is being taken to address the technical barriers that limit electrolyte performance for silicon-based anode systems. The PI will study the mechanism of improved capacity retention for Si nanoparticle electrodes in the presence of various electrolyte additives such as FEC and/or VC. The reviewer suggested that it would have been good if there were information regarding the experimental techniques. The reviewer was also concerned that contamination may happen when transferring the electrode sample to the scanning electron microscope (SEM), XPS, and Fourier Transform Infrared spectroscopy (FTIR) devices which may significantly change the results.

Reviewer 5:

The reviewer offered that the PI's strength is in their expertise of chemical synthesis, not for electrochemical chemical testing or surface physical analysis. It seemed to this person that the project was not sufficiently designed for leveraging the PI's strength.



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.**Reviewer 1:**

The reviewer reported that new high-performance electrolytes were identified and evaluated and that the work has concentrated on the study of the electrolyte composition and additives effect on the structure of the SEI on the silicon particles. The work has related to understanding the effect of the volume changes on charge and discharge on the anode performance. The reviewer explained that the effect of various electrolyte additives leads to greater stability and longer cycle life.

Reviewer 2:

The reviewer reported that the PI has studied the electrolyte with the addition of FEC and VC, and has performed electrochemical and ex-situ analysis for the anode surface. The reviewer indicated, however that limited information for the reaction mechanism was provided due to the lack of in-depth analysis (e.g., alternating current [AC] impedance).

Reviewer 3:

The reviewer affirmed that the investigator made good progress this past year. The cycling performance of electrolytes with different concentrations of added FEC and/or VC was investigated. The reviewer reported that the optimal electrolyte formulation for cycling Si anodes was found to be 10% FEC in 1.2 M LiPF₆ and 1:1 EC/DEC. Surface analyses of the electrodes were also performed using SEM, XPS, and FTIR.

Reviewer 4:

The reviewer pointed out that the team was recently redirected to study the SEI on Si anodes, so given the time spent on the project, only background work was completed that should become a foundation to addressing DOE goals. The reviewer reported that very interesting findings were identified on the mixture of FEC/MEC and the effect of Li salt/polymer ratio on the SEI stability needed to be systematically studied.

Reviewer 5:

The reviewer cautioned that it was not clear why the electrodes cycled with less additives had much less cracking. The reviewer emphasized that it was important to understand this problem so better electrolytes could be designed.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer described that the work has concentrated on developing a clear understanding of the effect of electrolyte additives on anode performance leading to developing the best electrolyte composition for the Si anode structure. The reviewer applauded the excellent cooperation; highlighting that samples supplied to other programs have added to the progress.

Reviewer 2:

The reviewer agreed that the collaboration was outstanding and that the team has had a good combination of people from academia and industry.

Reviewer 3:

The reviewer praised that the collaborators were well-suited for the research. The reviewer suggested that the PI should demonstrate the contribution of each collaborator.

Reviewer 4:

The reviewer recognized that the PI had assembled a good team of investigators to accomplish their goal. The reviewer detailed that the team includes members from BASF, LBNL (both the High-Voltage Spinel Focus Group and Silicon Focus Group), Yardney Technical Products, ANL, and the National Aeronautical and Space Administration Jet Propulsion Laboratory. The reviewer stated that this should ensure that the electrolyte being developed was the best material for the electrochemical couple that the DOE had been developing.

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.

Reviewer 1:

The reviewer explained that the future research would develop a mechanism for the interaction of the electrolyte on silicon anode materials on cycling, as well as a mechanism for capacity retention on cycling.

Reviewer 2:

The reviewer asserted the very good understanding of the challenges, particularly the reactions of the electrolyte with the surface of the lithiated silicon. It would be interesting to the reviewer to see if the researchers could do investigation on ex-situ pre-lithiated silicon anode to separate complex data interpretation based on the full cell studies.

Reviewer 3:

The reviewer noted that this was the final year for the project and that the work would be completed in the final months and a manuscript would be submitted for publication.

Reviewer 4:

The reviewer hoped that the authors at some point would propose a mechanism that would be able to explain the beneficial properties of added VC and FEC on the SEI. The reviewer highlighted that that should help in the guidance for future research.

Reviewer 5:

The reviewer proposed that the PI should focus on synthesis of new additives, salts, and solvents, and not on the physical and electrochemical analysis, which were not in the area of the PI's expertise.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer stated that high conductivity, stable electrolytes and high capacity anodes were critical to the use in batteries for powering automobiles.

Reviewer 2:

The reviewer agreed that the project supports the overall DOE goals and that electrolyte investigation is critical for the development of high energy Li or Li-ion batteries for transportation technologies.

Reviewer 3:

The reviewer confirmed that in order to meet DOE's goals, a new electrochemical anode such as Si will be necessary. Thus, according to the reviewer, it is highly-relevant to investigate electrolyte to determine the best system for cycling Si.

Reviewer 4:

The reviewer agreed that enabling advanced anode materials was necessary for EVs to succeed.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer commented that the total project funding appeared to be appropriate.

Reviewer 2:

The reviewer stated that the resources were adequate for the present work schedule.

Reviewer 3:

The reviewer commented that the PI should have focused on the chemical synthesis of new compounds either additives or salt or solvent, in which area the PI has adequate resource and expertise.

New Electrode Design for Ultrahigh Energy Density: Yet-Ming Chiang (Massachusetts Institute of Technology) - es071

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

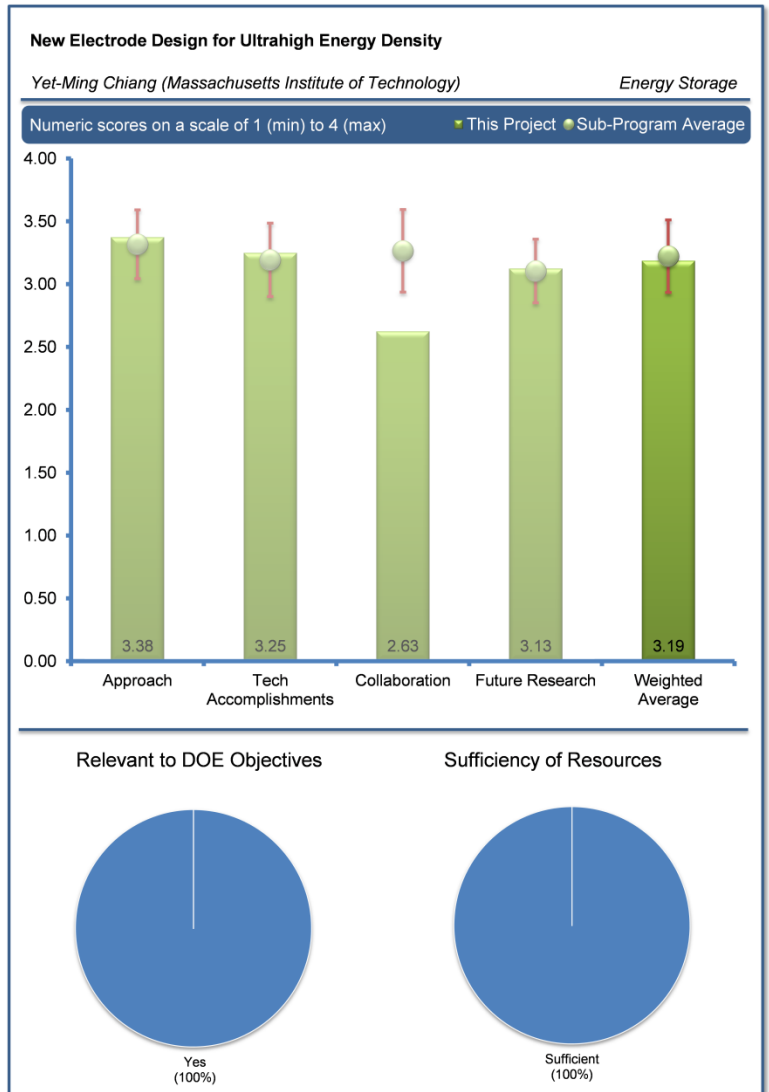
The reviewer remarked that this was a fascinating approach that may result in a nearly ideal electrode structure, promoting the ionic conductivity. However, it was not quite clear to this person on how to enhance the electronic conductivity for materials with low intrinsic electronic conductivity.

Reviewer 2:

The reviewer offered that this is an interesting and very innovative approach to make high aspect ratio electrode structures. Moreover, it would seem both easy to scale and relatively inexpensive. The reviewer noted the researchers' that the use of blocking electrodes and impedance to measure ionic and electronic conductivities is also very good. The reviewer also explained that the researchers were using a good filtering process to select those materials that could best benefit from this fabrication method and which ones to drop from consideration, rather than trying to force fit every material into their technique.

Reviewer 3:

The reviewer agreed that the approach to develop a more efficient electrode structure was important from a technical standpoint. The reviewer also anticipated that the likelihood of achieving higher energy density than with conventional structures is also excellent. However, the reviewer stated that complications of the process (LN₂ cooling, careful handling and control) may make the process too expensive for the cost goals of the DOE program. The reviewer suggested that it would be useful for the PI to begin to investigate modified processing to enhance the utility of the method; for example, the sintering step may not need to be as complete as presently done leaving some internal porosity that could conceivably be filled with an electronic conductor, at least to some extent. This would make the requirement of excellent conductivity of the base material less important, although it would compromise to some extent the electrode loading. At present, it appeared to the reviewer that 10 times the conventional loading could be achieved with this technique (as shown for LCO), but perhaps five times the loading would still represent a major step forward in improving energy density. The reviewer noted that the PI alluded to this in the remaining barrier slide where they discussed the results of calculations showing the need for microporosity in the lamellae.



Reviewer 4:

The reviewer agreed that increasing the area capacity through electrode thickness was a great approach to impact battery specific energy and energy density. The reviewer also noted that being able to eliminate binders and carbon additives was an added advantage which the reviewer stated the PI has some unique ideas to accomplish this. While the concepts are unique, there did not seem to this reviewer to be any cost-benefit analysis to these studies. The reviewer recounted that the primary issue with thick electrodes was the current distribution throughout the electrode during constant current discharge; specifically, the electrolyte cannot support the current. The reviewer criticized that there did not seem to be a plan, at least this year, to discharge the electrodes at significant C-rates (i.e., C/3 and higher). The reviewer also indicated that because there was not any conductive carbon additive and that these oxides did not have a high electronic conductivity, the PI was correct to be concerned about electronic conductivity effects.

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.**Reviewer 1:**

The reviewer stated that it would be more interesting to see the performance as the electrode, particularly the cycle life, since it is questionable how robust the structure is upon cycles in which the electrode material undergoes expansion-contraction cycles. The reviewer highlighted that the enhanced ionic conductivity can be obviously expected for such a structure. The reviewer also cautioned that the current data concerning the capacity at the low rate is not impressive.

Reviewer 2:

The reviewer indicated that the PI had shown excellent results to date with the good conducting LCO. The reviewer also reiterated that the poorer conducting NCA would clearly need thinner lamellae as discussed by the PI. The project person described that the methodology had also allowed the measurement of intrinsic properties such as electronic conductivity, ionic conductivity and tortuosity.

Reviewer 3:

The reviewer observed that the PI spent a lot of time measuring conductivity and diffusion rates in the solid active material phase of the electrodes; while these were important values, it was more important to see what C-rates the thick electrodes will support. Also, the reviewer did not see what electrolyte the PI was using, but noted that the transport of Li ions in the electrolyte did not seem to be important to the PI.

Reviewer 4:

The reviewer described that the researchers have successfully used the method to make pillar-like electrodes that have very low tortuosity. The reviewer pointed out that the researchers' measurements of the change in conductivity and ionic diffusivity for NCA as a function of state of charge was also very worthwhile, however this person was not sure how new this information actually was. The reviewer also indicated that the initial samples did not show the rate performance the researchers were going after, but acknowledged that there was a plan to reach the targets.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer would have liked to see some collaboration developing between the group and either a national laboratory group interested in battery engineering or an industrial partner.

Reviewer 2:

The reviewer agreed that the researcher probably did not need much collaboration for now, but if successful, that this would need to be brought into the cell validation program at ANL. The reviewer recognized that not every project needed a lot of collaboration, so did not see why this is factored into a total score.

Reviewer 3:

The reviewer simply indicated that the PI had a few collaborations.

Reviewer 4:

The reviewer agreed that it was very important to examine the electrochemical performance.

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.

Reviewer 1:

The reviewer requested that the researchers show more electrochemical data including the rate capability.

Reviewer 2:

The reviewer voiced that the focus on the critical barriers seemed to be developing. The reviewer proposed that additional considerations, such as suggested in the review on the approach could be quite helpful.

Reviewer 3:

The reviewer agreed that the PI had a good plan that included testing to the United States Advanced Battery Consortium (USABC) protocols and starting work on a negative electrode.

Reviewer 4:

The reviewer reported that the researchers planned to try and go thinner and also to thin the space between the electrode pillars to permit the electrolyte to penetrate.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer asserted that intrinsic energy density of materials could be greatly enhanced by clever electrode structures such as this work.

Reviewer 2:

The reviewer explained that this work, if successful, promised to yield thick electrodes that could also be charged and discharged at high rates, which addressed a critical factor in trying to achieve both high energy and high power for HEV and PHEV cells. The reviewer also stated that, as the researchers were aware, the method may be somewhat limited to materials that are good or at least not bad electronic conductors.

Reviewer 3:

The reviewer agreed that overall, the project was very relevant.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer stated that, based on the productivity of the PI, sufficient resources seemed to be available.

Interfacial Processes in EES Systems Advanced Diagnostics: Robert Kostecki (Lawrence Berkeley National Laboratory) - es085

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer described that, in general, the PI applies spectroscopic techniques in-situ and ex-situ in conjunction with electrochemical studies to examine the SEI on pertinent electrode materials. The reviewer stated that the PI has been conducting these studies for many years and generally has expanded the diagnostic tools.

Reviewer 2:

The reviewer commented that the use of spectroscopic methods to study the interfaces of active materials to infer the direction of parasitic reactions is well-developed. The reviewer would like to see some more detail, however, on the approach used in this contract. The reviewer asserted that many of the slides were very general and similar to those of the previous year.

Reviewer 3:

The reviewer described that many spectroscopic and imaging techniques were applied to examine electrode materials; however, no clear understanding and goals appear to have been defined.

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.

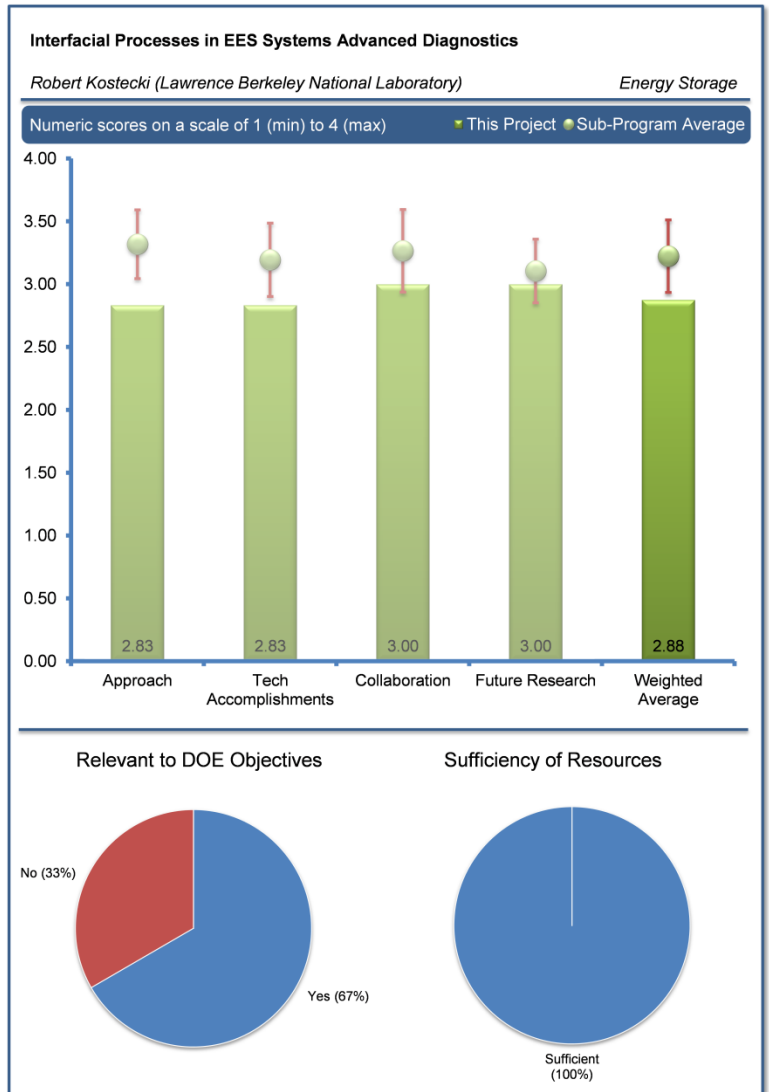
Reviewer 1:

The reviewer found the PI's studies using fluorescence unique and worthwhile. The reviewer also said it will also be interesting to see where the PI goes with the Li alloy studies.

Reviewer 2:

The reviewer criticized that lots of data were thrown in, but the project did not provide new findings beyond information that was available in the literature. The reviewer also expressed that in the SEI layer that contains products of electrolyte oxidation by oxidized transition metals (e.g., Mn(IV) and Ni(IV) during charging), the presence of Ni(II), Mn(II), and Mn(III) were easily expected.

The reviewer also criticized that the interpretation of some data (Slide 19) was not convincing, for example the electrode size was not specified, but currents instead of current densities were plotted. Thus, it was not clear if the peaks were due to surfaces or bulks. The reviewer offered that, rather than oxidation of electrolyte, the reduction peaks can be due to reduction of surface oxides. This person also asked if there was any Li UPD on Sn. The reviewer concluded by asking what new findings or contributions were accomplished.



Reviewer 3:

The reviewer stated that the accomplishments seemed to be mainly a continuation of the previous year's studies, as shown by the similarity of the presentations. It was not very clear to this reviewer what had been accomplished in the current year.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer simply stated that the researchers presented a good research network.

Reviewer 2:

The reviewer indicated that the collaborations were good, but the reviewer would like to see some stronger interaction with electrochemists working on EV battery problems to keep the work grounded.

Reviewer 3:

The reviewer stated that the PI had a few collaborations outside the organization.

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.

Reviewer 1:

The reviewer commented that the degradation of the high-voltage spinel is due to the reaction associated with electrolyte and instability of the material itself (e.g., oxygen evolution from decomposition). The reviewer asked what the SEI poisoning was and requested that the researchers please show how the high-voltage spinel is "poisoned" because this was not clear. The reviewer asked if the SEI layer is slowing down the charge-discharge processes. The reviewer suggested using more practical approaches and clear data presentations for better and wider contributions.

Reviewer 2:

The reviewer observed that the future work was practically identical to 2013.

Reviewer 3:

The reviewer commented that the PI was proposing to continue these studies; specifically, that the PI was going to attack several challenging problems.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed that the relevance of this work was clearly demonstrated.

Reviewer 2:

The reviewer observed a lack of focus and commented that too many different techniques were thrown in; lacked a focus.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer stated that, based on the productivity of the PI, the funds were sufficient for the project.

Reviewer 2:

This reviewer admitted to not having a clue.

Predicting and Understanding Novel Electrode Materials from First-Principles: Kristin Persson (Lawrence Berkeley National Laboratory) - es091

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

This is an excellent use of computational modeling to understand the key problem inherent in the Li_2MnO_3 cathode material, in the opinion of this reviewer, and a good use of activation energy to estimate the likelihood of a reaction actually occurring versus just looking at the thermodynamic driving force.

Reviewer 2:

The reviewer considered investigation of Mn migration from the Mn layer to the lithium (Li) layer to be very important and critical to understanding the mechanism of failure in these types of cathode powders. It will be a big plus if the research can be expanded further so that these results are used as guidance for the experimentalist, the reviewer said.

Reviewer 3:

The reviewer found the approach very interesting and felt that the results provided good insight into the structural evolution with charge-discharge cycles. However, the reviewer noted, this computational study is based on the bulk structures, while many electrochemical aspects of the material's behavior in the LIB environment are dominated by the SEI layers.

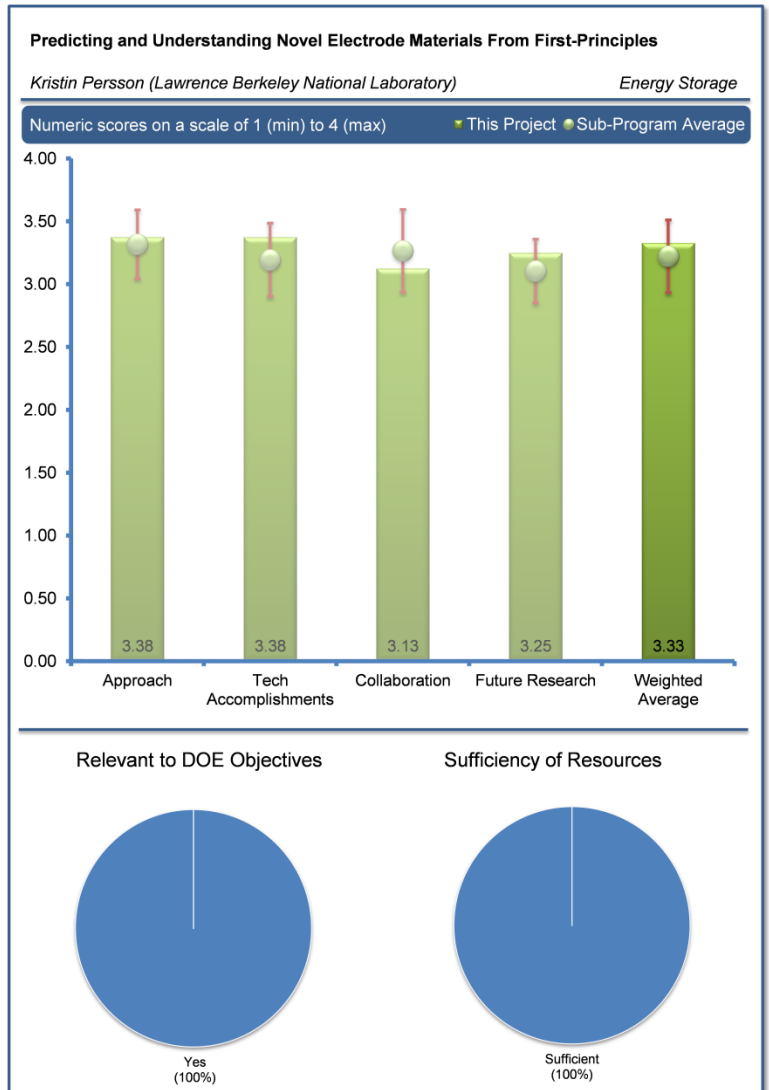
Reviewer 4:

The reviewer said the PI's approach to theoretical examination of Li_2MnO_3 during cycling to determine the implications for lithium- and manganese-rich (LMR) electrode materials was a good idea at the time. Recent experimental evidence, however, seems to indicate Li_2MnO_3 domains in LMR-NMC cycle behave quite differently from the pure compound.

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.

Reviewer 1:

The reviewer found it difficult to correlate the computational results of Accomplishment 4 with experimental results, since the experimental results are for the material with x greater than one and the phase separation in the calculation occurs at less than 1. Trapping Mn in the Li layer appears to be reversible according to calculations, the reviewer observed, since the Mn defects are no longer favorable in energetics at $x=1$, which does not explain the voltage fade. Identifying the possible migration paths should be useful in considering degradation mechanisms, the reviewer concluded.



Reviewer 2:

The PI has several interesting results concerning overall structural stability and manganese migration, the reviewer said.

Reviewer 3:

The reviewer urged that the dumbbell path be investigated further, since it seems to be a fairly new phenomenon. Further understanding of this pathway is desirable, the reviewer said, to see if it represents a new variable by which Mn migration can be suppressed.

Reviewer 4:

The reviewer expressed the opinion that this modeling effort basically explains that manganese migration into the lithium layer at high states of charge is the main issue related to the fade of this material in cells and called this finding absolutely critical. It is very hard, the reviewer observed, to solve a problem without being clear about its true nature and this work provides that knowledge. The reviewer elaborated with the observation that this work suggests surface treatments are unlikely to make any improvement in cycle life for this material. Discussions with other PIs, the reviewer said, suggest this is indeed the case for pure Li_2MnO_3 , but the Envia Systems work shows advantages for atomic layer deposition (ALD) on the mixed layered material. So it appears that the findings of this work perhaps address only one of the degradation mechanisms of the layered-layered material. The reviewer found it interesting that the mechanism defined is counterintuitive in that the oxygen changes oxidation state rather than the transition metal ions.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer said it was good to see collaboration with experimentalists.

Reviewer 2:

The reviewer noted that the project has a few collaborations outside its own organization.

Reviewer 3:

Important collaborators are in place, the reviewer said, in particular with experimentalists.

Reviewer 4:

The reviewer was unsure if this project required much collaboration to run the modeling, but was unwilling to mark the project down for lack of collaboration, despite knowing that the Annual Merit Review (AMR) rating system calls for that. The reviewer urged that this work be disseminated and leveraged by the experimentalists in the DOE community, but had the impression others were unaware of it or perhaps unpersuaded because it is only modeling. The reviewer considered it very important that experimentalists follow up on any new insights this work generates on possible solutions, but was concerned that this might not happen unless the work were more widely reviewed and critiqued within the DOE program. This concern was somewhat moderated by the Envia Systems presentation in which this modeling work was at least acknowledged, the reviewer said, although it seemed it had been ignored by the Argonne group. If there is a disagreement, the reviewer went on, resolve it as a team using science, logic and data. Perhaps the PI needs to force the issue, the reviewer concluded, but in any case, management should ensure they fully capitalize on good work such as this.

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.**Reviewer 1:**

The reviewer wondered if it would be possible to look at the SEI layers.

Reviewer 2:

Noting that the PI is moving to study LMR-NMC materials, the reviewer said it will be interesting to see how the composite structure is approached.

Reviewer 3:

Deeming future research plans excellent, the reviewer described the next steps as attempting to determine whether Mn migration can be blocked by using dopants to pin the Mn in place and prevent the structural change. In essence, the reviewer said, leverage their new-found knowledge and the ability to rapidly model the effects of such doping on the stability of the structure. The reviewer recommended that any success in this area be prioritized by experimentalists to see if it really works.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The PI's work is very relevant, the reviewer said, although a great case for its importance had not been made.

Reviewer 2:

This work addresses one of the most important issues facing implementation of the high energy cathode Li_2MnO_3 that forms part of the layered-layered cathode material.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer wondered if all computations are carried out by the presenter or if the presenter needs additional hands.

Reviewer 2:

Based on the PI's productivity, the reviewer said, funds are sufficient to support the effort.

Studies on High-Energy Density Lithium Ion Electrodes: Jagjit Nanda (Oak Ridge National Laboratory) - es106

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

In the opinion of the reviewer, the program entails a comprehensive but excessively ambitious approach to solving far too many problems, including a new synthesis of high-capacity cathode, which by itself is a huge project.

Reviewer 2:

The reviewer cited some project aims, including developing methods and diagnostic techniques such as Raman mapping, x-ray absorption near edge spectroscopy (XANES), etc. and studying surface morphology/structure on LMR-NMC cathode materials to better understand capacity loss on cycling. The reviewer noted that transmission x-ray microscope (TXM)-XANES studies revealed changes in the Mn oxidation state that correlate with voltage fade.

Reviewer 3:

The reviewer said that the approach seemed to be feasible and is consistent with the overall program goals, but deemed the effort rather diffuse, noting that it ranged from material-related studies (bulk to interface), with electrolyte additives and surface coatings, to multi-electron cathodes. The reviewer listed the project objectives as including utilization of new diagnostic techniques to understand the life-limiting mechanisms of high-voltage cathodes, including the local inhomogeneities and correlating performance with the material properties (crystal structure and morphology; evaluating high-voltage electrolyte additives and solid electrolyte coatings (LiPON) for improving the cycle life of LMR-LLC cathodes; and designing new syntheses of high-capacity cathodes. The reviewer remarked the use of Micro-Raman mapping to monitor the inhomogeneity in state-of-charge during cycling, and X-ray imaging and spectroscopy (XANES) for three-dimensional elemental mapping and tomography of cycled LMR-NMC cathode particles.

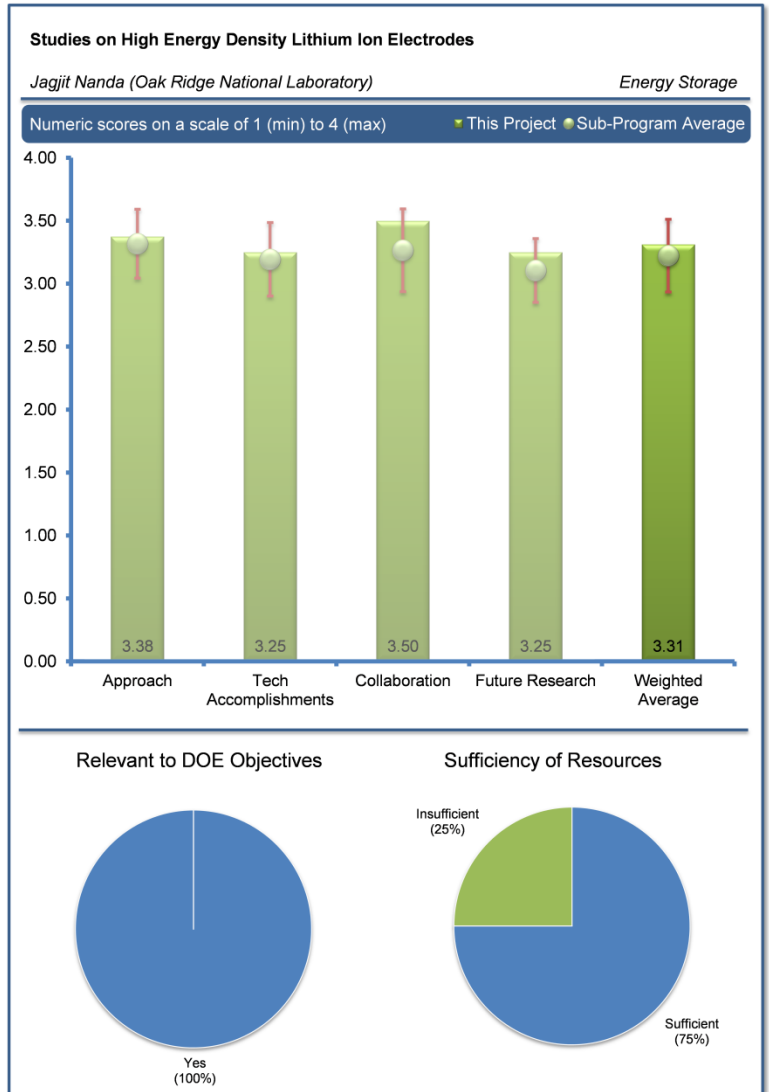
Reviewer 4:

The reviewer noted that different image techniques were used for mapping particle morphology and valence state and found the tomographic reconstruction using XANES particularly interesting.

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.

Reviewer 1:

Overall, the reviewer said, the progress is good and consistent with the DOE goals. There were some interesting and useful accomplishments presented in understanding the bulk and morphological changes in the LMR-LLC cathodes, the reviewer went on.



Noting that correlation of the oxidation state of TM cations (manganese) to the onset of voltage is not new, the reviewer nonetheless pointed out that it substantiates the findings of previous DOE researchers, although the results are not entirely consistent. To support that observation, the reviewer noted that these results point to the decrease of all three TM concentrations in the surface, contrary to Zhang's finding of surface-enrichment of reduced Ni. The reviewer also found the use of micro-Raman mapping interesting, but questioned the conclusion of PF₆⁻ intercalation at less than 4.8V into carbon (diluent). The study with LiPON the reviewer judged to be promising and approved of its being scaled up. The reviewer felt that some questions from previous reviewers on the efficacy of coating electrode vs. particle had not been properly answered. The benefit from various high-voltage electrolyte additives on cycle life the reviewer called encouraging, but wondered what the electrode loadings were and cited the need for them to be comparable to the current values for NCA cathodes. The performance of multivalent cathodes, the reviewer felt, is too preliminary to permit an assessment.

Reviewer 2:

It is not expected that additives will solve the cycle-life/voltage fade issues, the reviewer said, since they are not predominantly related to surface phenomena. The reviewer then inquired about justification for all the work on additives. The PNF-2 additive apparently looks good, the reviewer said. The diagnostic work using XANES tomography, in the reviewer's judgment, appears quite informative and will certainly help to expand our knowledge about the failure modes of these cathodes. SOC-dependent analytical studies are also novel. But in general, the reviewer concluded, there is nothing significant in this cathode work, as multiple groups are working on these types of low-voltage cathodes and the uniqueness of each approach is not obvious.

Reviewer 3:

Changes in the oxidation state of Mn on cycling have a strong correlation with voltage fade on cycling, the reviewer stated. Also, the change in morphology-oxidation state of cathode particles on cycling gives rise to a change from spherical to an oblong particle, the reviewer observed questioning, and cathode materials with capacity of over 200 mAh/g were synthesized.

Reviewer 4:

The result of electrolyte additives was not surprising, the reviewer said. New cathode material Li₂Cu_{0.5}Ni_{0.5}O₂ showed poor cyclability and a poor voltage profile, the reviewer observed.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer called the team a great collaborative team.

Reviewer 2:

There has been a strong, deliberate effort to coordinate with the Army Research Lab (ARL), ANL, LBNL, Ford Motor and Tennessee Tech on various parts of this activity, the reviewer said.

Reviewer 3:

There are good, ongoing collaborations with the other DOE laboratories, a university, and Department of Defense (DOD) researchers, the reviewer said.

Reviewer 4:

The reviewer observed that the project team works with ARL on electrolytes.

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.**Reviewer 1:**

The reviewer expressed the opinion that the project should still be on novel diagnostic studies and less on these LiMM'O₃ compounds, which in the reviewer's view, show very little promise.

Reviewer 2:

The reviewer summarized the future work by noting that it will include Raman and X-ray (XANES) studies to correlate state-of-charge phenomenon with changes in NMC cathode materials, and that high-voltage additives to the electrolyte will be evaluated for their effect on charge retention. Under continuous high-voltage cycling, the reviewer observed, the LMR and LMC particles undergo a change in morphology and that it has been found that the surface structure of the cathode particles changes.

Reviewer 3:

Overall, the reviewer said, future plans are consistent with the overall goals of the advanced battery research (ABR) program. The reviewer cited three tasks in the proposed future research, the first of which is continuing development of high-capacity, 4-Volt lithium-ion cathodes ($\text{Li}_2\text{MiMiO}_2$ and $\text{Li}_2\text{MiMiiO}_3$, where Mi and Mii are Ni, Cu, Fe, or Cr) by incorporating an isovalent or supervalent dopant to stabilize the structure upon the extraction of second lithium. The second is local state of charge (SOC) and characterization studies on the cycled electrodes, and the third is utilizing electrochemical impedance spectroscopy (EIS) to monitor the growth of surface films upon cycling. The reviewer suggested focusing more on the first two topics, as the third topic is more general and is being pursued by others in ABR.

Reviewer 4:

The reviewer felt it is unclear what the advantages are of using full-cell, since EIC can also be performed from a half-cell. When a full-cell is used, the reviewer asked, how the contributions of the anode and cathode can be distinguished.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The work is definitely important from the standpoint of DOE's objectives, the reviewer said, since a good understanding of the failure mechanism is critical in developing high-energy, low-cost batteries for automotive applications.

Reviewer 2:

The work is at the cutting edge of the need for higher-performance cathode materials, the reviewer declared, and the rate of progress is outstanding.

Reviewer 3:

High specific energy, long cycle life and low cost are the performance drivers for Li-ion batteries in electric vehicles, the reviewer said, and LMR-LLC cathode materials are promising due to their high capacities at high voltages, and possibly their low cost owing to high Mn contents. However, the reviewer went on, their performance degradation upon cycling, both in capacity and voltage, is an impediment to their use in Li-ion cells. This project is aimed at understanding and mitigating these failure modes, the reviewer concluded.

Reviewer 4:

The reviewer simply stated to develop high capacity and high voltage cathode for Li-ion batteries.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer, deeming project resources insufficient, said that consideration could be given to increasing the funding for this team given the broad scope of the program.

Reviewer 2:

Resources are barely adequate for the proposed program, the reviewer said. An increase in funding would allow widening the study with appropriate speed in arriving at the best cathode composition, the reviewer went on, and urged that such an increase be considered.

Reviewer 3:

The resources are adequate for the scope of the project, in the opinion of this reviewer.

Development of Computer-Aided Design Tools for Automotive Batteries: Steven Hartridge (CD-Adapco) - es118

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer termed this project (noting that it is now nearing its end) one of the essential building blocks in computer aided engineering (CAE) tool development. If further work is awarded, the reviewer recommended, it should depart from the spirally wound cell variants and incorporate large-format cell variants with boundary conditions of design intent for pack level performance, including safety stability. The reviewer concluded by saying that this was a great approach to identifying lithium loss and SCI layer development.

Reviewer 2:

The reviewer observed that CD-adapco and Battery Design LLC, working together, have created a computer aided design (CAD) tool to aid in reducing the time/cost for battery design. The work began with the creation of electrochemical and thermal models, which then led to cell-level and pack models, the reviewer went on, while electrolyte data was input from an electrolyte model developed at Idaho National Laboratory (INL). The cell models and overall CAD tool were, or are being, tested by National Renewable Energy Laboratory (NREL) and Oak Ridge National Laboratory (ORNL); cell performance was provided by JCI (Johnson Controls, Inc.) and perhaps A123 Systems, the reviewer concluded. However, the reviewer said, it is unclear what validation has been made for the property inputs or what these are, specifically.

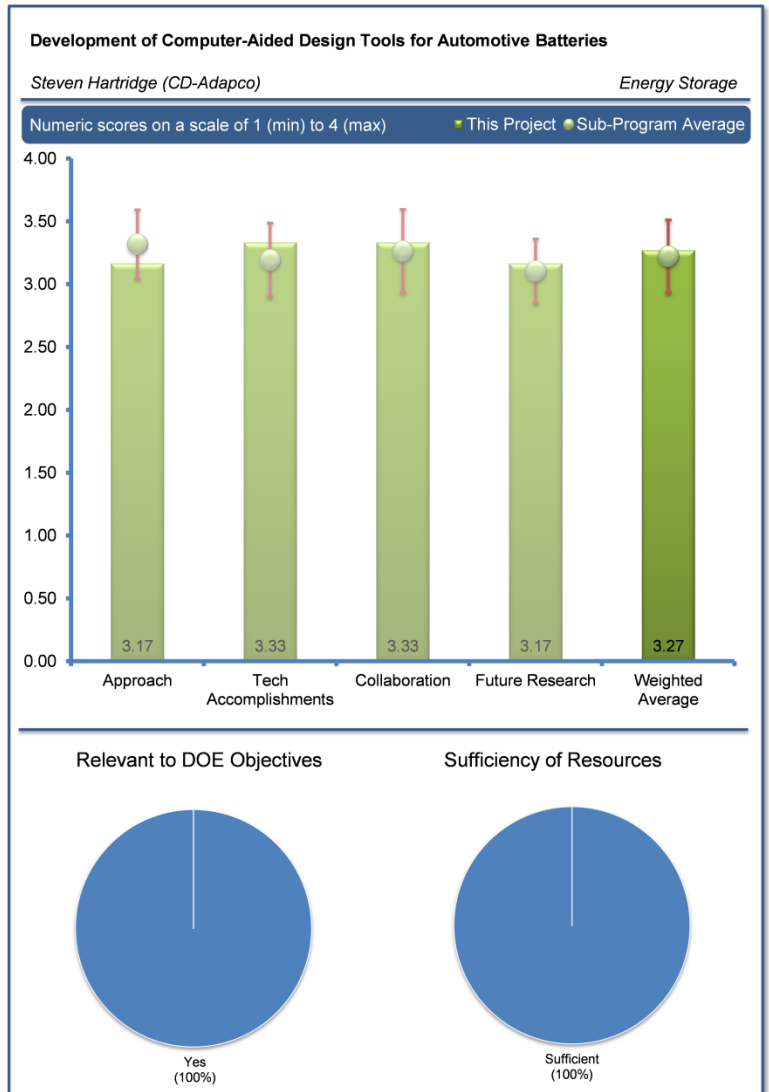
Reviewer 3:

The project team proposed using separate electrochemical and thermal models to predict performance and life, the reviewer noted. Their models were not coupled and seemed to be empirically based, since it required iterative fitting of parameters, the reviewer added, thus, the applicability of the models to cells not manufactured by JCI or A123 Systems is unclear. The reviewer felt the team need to show how their materials database was used in their models.

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.

Reviewer 1:

The milestones, the reviewer noted, indicate that ORNL was to validate the open architecture compatibility by May 2014. No information was provided during the presentation with regard to the results of that validation testing, the reviewer said, and without significant



validation, the utility and reliability of the CAD tools will be very limited. The project seems to rely on electrolyte data obtained from Gering's (Idaho National Laboratory) electrolyte model, the reviewer noted, and while this is perhaps understandable given the limited amount of rigorous electrolyte property data available in the scientific literature, but a model based upon a model may have severe limitations. Very little validation data, and no blind tests that the reviewer was aware of, have been openly reported for Gering's model. Thus, the reviewer said, the accuracy of Gering's model remains questionable to an external observer. The reviewer was left with two questions and asked what electrolyte properties were required for the CAD tool and could these be determined experimentally in a straightforward manner; and how dependent on or sensitive to specific material properties were the results of the CAD tool. Some validation via a comparison of tool results and experimental data was provided in the Technical Approach slides, the reviewer noted, but felt that does not conclusively demonstrate the CAD tool's validation.

Reviewer 2:

The data showed good correlation between the measured voltage and the modeling results on the cell types specified in the project team's accomplishment table, the reviewer said. However, since their model was empirically based, the reviewer felt the applicability of the models to other cells not specified in that table was not clear.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

This program collaborated with the well-respected expertise of A123 Systems and JCI, the reviewer said, but there is always room for involvement by many more cell and battery developers, although, the reviewer added, that this is perhaps too difficult to be practical. There is the fundamental paradox, the reviewer noted, that all these cells are quite different by many metrics.

Reviewer 2:

JCI has evidently been very open with input data for the CAD tool, which has greatly facilitated its development, the reviewer observed. JCI provided various cells and performed the experimental testing for CD-adapco and Battery Design, LLC. Likewise, the reviewer said, A123 Systems provided pouch cells to extend the CAD tool evaluation to cells of that type, since the tool was developed for spirally wound cells. The reviewer felt it was unclear how open A123 Systems had been with data input. NREL and ORNL are noted to be collaborating with CD-adapco and Battery Design LLC to create an open architecture software framework to enable model transfer between CAEBAT projects, the reviewer said, but no information was provided regarding how far this has progressed. Nonetheless, overall the collaboration appears to be highly fruitful, the reviewer concluded.

Reviewer 3:

The intention to use JCI and A123 Systems to validate the results was good, the reviewer felt, but it seemed their participation was mostly limited to testing coordination rather than to validation testing.

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.**Reviewer 1:**

The reviewer referred to earlier comments, which this reviewer stated was well recognized by the presenter.

Reviewer 2:

No future work was mentioned, as the project will be finalized in July 2014, the reviewer noted, but the major milestones for the project appeared to have been met.

Reviewer 3:

No future work was presented the reviewer observed because the project was 90% complete.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The program to develop computer-aided design (CAD) tools for transportation batteries is well-founded, in the reviewer's judgment. Much of the technology and design development for transportation batteries has matured and CAD tools, the reviewer predicted, will likely be the key to future design improvements and manufacturing cost reductions. The work may also provide additional insight into fundamental science needs for battery materials, the reviewer speculated.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

With the project coming to an end, the reviewer said, CD-adapco and Battery Design LLC appear to have accomplished the goals laid out for the project, suggesting that they did have adequate resources (with collaborations) for the work.

Development of Computer-Aided Design Tools for Automotive Batteries: Taeyoung Han (General Motors LLC) - es119

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

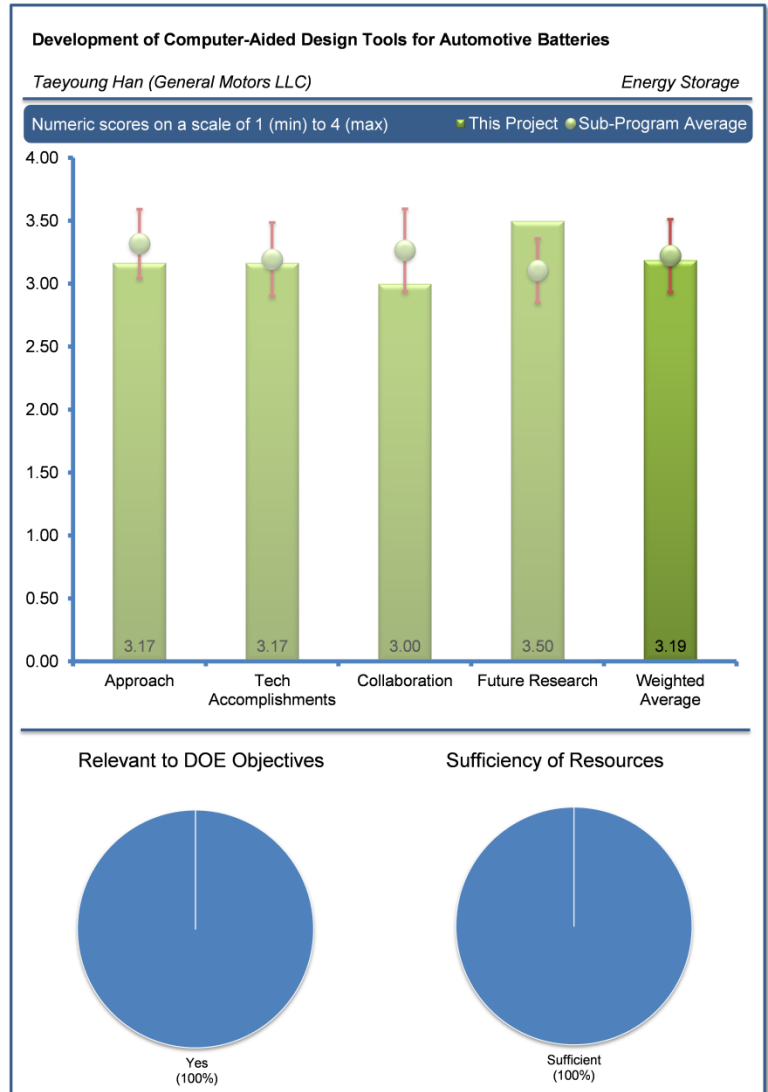
The reviewer expressed a desire to have seen more technical details of the models used, especially the underlying physics and chemistry of the batteries and how they are simulated.

Reviewer 2:

The project, the reviewer noted, has developed a cell-level model which is now being developed into a full pack-level model. Reduced-Order Models (ROMs) are used for the flow and thermal analysis at the pack-level. The strategy, the reviewer said, is to develop a range of methods which will permit trade-offs between computational expense and resolution.

Reviewer 3:

The project team proposed to use the ANSYS ABDT tool to simulate electrochemical and safety performance at the cell and pack level, the reviewer observed, with ROM used to simplify the computation time, at the expense of accuracy.



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.

Reviewer 1:

Significant progress seems to have been made for the model and many of the difficulties clearly identified, the reviewer said. However, no information was provided about the material properties inputs for the models. The reviewer was left with asking questions on this aspect of the project including how these are being experimentally determined or if they are estimates; how sensitive the models are to these input parameters; and if blind evaluations have been conducted as part of the verification process. The reviewer cited accomplishments of the project including the official release of ANSYS (Version 15) to the public in December 2013 and completion and validation of a system-level model without ROM (comparison of full field simulation with test data), which demonstrated the system's simulation for the US06 drive cycle. Development of a linear (LTI) ROM model, the reviewer noted, is in progress, but challenges remain, as some features required for the models are in fact nonlinear.

Reviewer 2:

Data showed good correlation between the measured temperature and the modeling results, the reviewer noted, but it did not seem that the electrochemical and thermal models were coupled, which the reviewer felt might have contributed to some of the errors. No simulation data on life was presented, the reviewer concluded.

Reviewer 3:

Progress toward development of a battery management system (BMS) does not seem to have been initiated yet, the reviewer observed.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer skipped the slide that discussed collaboration.

Reviewer 2:

The reviewer cited General Motors' (GM) work with Ansys and Esim to develop the models; NREL's technical direction and cell chemistry model for multiple particle/active materials; ORNL's provision of the Open Architecture Software and GM's conduct of the mathematical model verification and cell/pack-level validation.

Reviewer 3:

The reviewer said that there is good collaboration with various teams and noted that their specific roles were described. However, the reviewer would have liked to see more validation data from independent testing by one of the collaborators.

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.**Reviewer 1:**

The reviewer noted that implementation of an already-developed thermal abuse/runaway model will be done to address thermal propagation within the pack and that practical cell cycle life models have been defined and will be added in the third quarter of 2014. A physics-based cycle life model will be added in the fourth quarter, the reviewer added. Work flow automation for the LTI/LPV ROM process will be completed and models will be implemented for multiple particle materials, since most commercial battery manufacturers are using multiple active materials in the cathodes and anodes, the reviewer went on and pack-level validation as well as other tasks will continue. All these are well-aligned with the project goals, the reviewer stated.

Reviewer 2:

Although the project team planned to finish the physics-based life model by December 2014, the reviewer said, no preliminary life data were shown.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The program to develop computer-aided design (CAD) tools for transportation batteries is well-founded, in the reviewer's judgment. Much of the technology and design development for transportation batteries has matured and CAD tools, the reviewer predicted, will likely be the key to future design improvements and manufacturing cost reductions. The work may also provide additional insight into fundamental science needs for battery materials, the reviewer speculated.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The project seemed to have sufficient resources, the reviewer said. Some difficulties have been identified, but these are not due to limited resources, in the reviewer's opinion.

Development of Cell/Pack Level Models for Automotive Li-Ion Batteries with Experimental Validation: Christian Shaffer (EC-Power) - es120

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer would have preferred to see more of a technical description of the physics and chemistry of degradation that were incorporated to accomplish the lifetime simulations.

Reviewer 2:

The reviewer listed the accomplishments of the project, including development of an electrochemical/thermal (ECT)-coupled cell and physics-based pack model and creation of a materials database to support the models for commercially relevant materials, which are claimed to be accurate over a wide range of temperatures, SOC, etc. Evidently, the reviewer said, this used thousands of coin cells to obtain high-quality material properties. The ECT3D software was integrated with the CAEBAT Open Architecture Standard (OAS), the reviewer concluded.

Reviewer 3:

The reviewer noted that the project team proposed to use the Electrochemical-Thermal Coupling (ECT) model to predict life. The ECT, the reviewer felt, should be predictive since it is not empirically based, but based on parameters extracted from the extensive materials database.

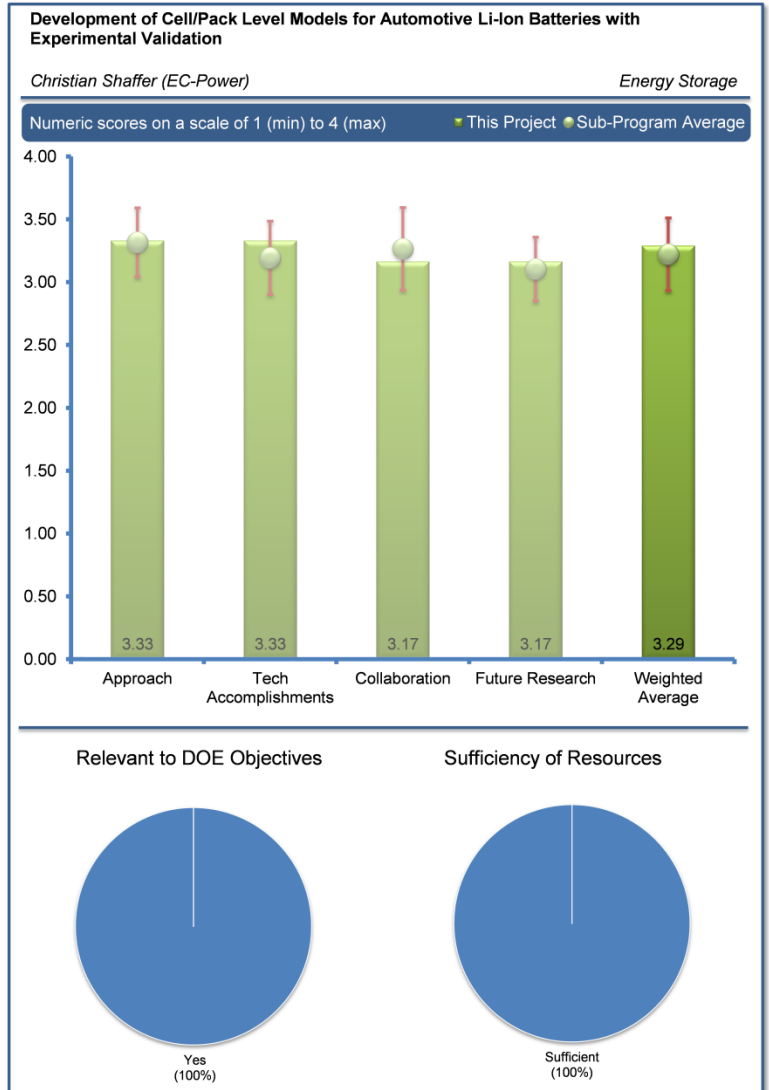
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer said it looked like good model verification had been accomplished for many technical features.

Reviewer 2:

The reviewer found validation/performance testing to obtain data on the temperature distributions and cycle life of cells quite interesting, but it was not clear what the results were from the Ford and JCI testing/validation of the models, except for the commercial cell external short data, which was compared with JCI data. What inputs, the reviewer wondered, are required for the models in terms of material properties, and if these are all now readily available from the materials database created. Further, the reviewer asked if this database will be available to other researchers. The presentation summary, the reviewer noted, indicates the software is commercially available and has been for several years. The project, in the reviewer's opinion, therefore seems to be one devoted to validation of an existing or recently updated model. Finding nothing wrong with this, the reviewer nonetheless found it unclear how well the model performs and what its limitations are (i.e., how thoroughly it has been validated and whether blind evaluations have been done).



Reviewer 3:

Data showed good validation between actual performance and simulation results at various rates and temperatures, the reviewer noted, and there was also good validation between actual life data and simulation results during early life. There was more deviation at later life, the reviewer observed, which discrepancy was attributed to error on the graphite anode. Good agreement on temperature rise was obtained in the nail penetration test with simulation data, the reviewer said.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

Noting that the project is led by EC Power with additional contributions from the following: NREL, the CAEBAT Program Administrator; ORNL, who provides the Open Architecture Software; Pennsylvania State University for materials testing and model validation; and Ford Motor Co./JCI for testing, validation and feedback. The reviewer said this seems to be an effective partnership, but said little information was provided regarding how the collaboration has worked out.

Reviewer 2:

The reviewer deemed there to have been good collaboration with various teams, whose specific roles were described. However, the reviewer would like to have seen more validation data from independent testing by one of the collaborators.

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.

Reviewer 1:

This project's completion date has already passed, the reviewer noted, but the work has been extended for a few extra months to finalize the deliverables.

Reviewer 2:

The reviewer noted that the project is near completion and most future work is focused on finishing up the reports, but expressed approval of the team's recommendation to refine the life model to gain accuracy, especially for longer life at high temperatures.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The program to develop computer-aided design (CAD) tools for transportation batteries is well-founded, in the reviewer's judgment. Much of the technology and design development for transportation batteries has matured and CAD tools, the reviewer predicted, will likely be the key to future design improvements and manufacturing cost reductions. The work may also provide additional insight into fundamental science needs for battery materials, the reviewer speculated.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer felt it was unclear that resources were indeed sufficient, but assumed so in the absence of other information.

Open Architecture Software for CAEBAT: Sreekanth Pannala (Oak Ridge National Laboratory) - es121

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

According to this reviewer, great emphasis was given to existing methods and pursuit to Open Architecture. The reviewer also observed the use of well-defined macro (thermal, electrical, mechanical) environment with a diversity of approaches and numerical methods.

Reviewer 2:

This reviewer recounted that the goal of this project is to create open architecture software to facilitate the integration of battery models for improved battery design. Standardized interfaces and file formats are used to provide access to commercial and public software. The reviewer summarized that the Open Architecture Software is being used for several of the other CAD projects within CAEBAT.

Reviewer 3:

This reviewer noted that a common standard is needed to compare the different battery models. However, to this reviewer, it was not clear why there was a need to integrate different battery models. Per Slide 4, each of the three commercial software suites is fully capable of battery simulation. There is a bigger need to benchmark the three commercial software suites to compare their accuracy than to integrate them. In addition, since the commercial software contains proprietary components, it was not clear to the reviewer the extent that those proprietary components could be shared for the integration effort.

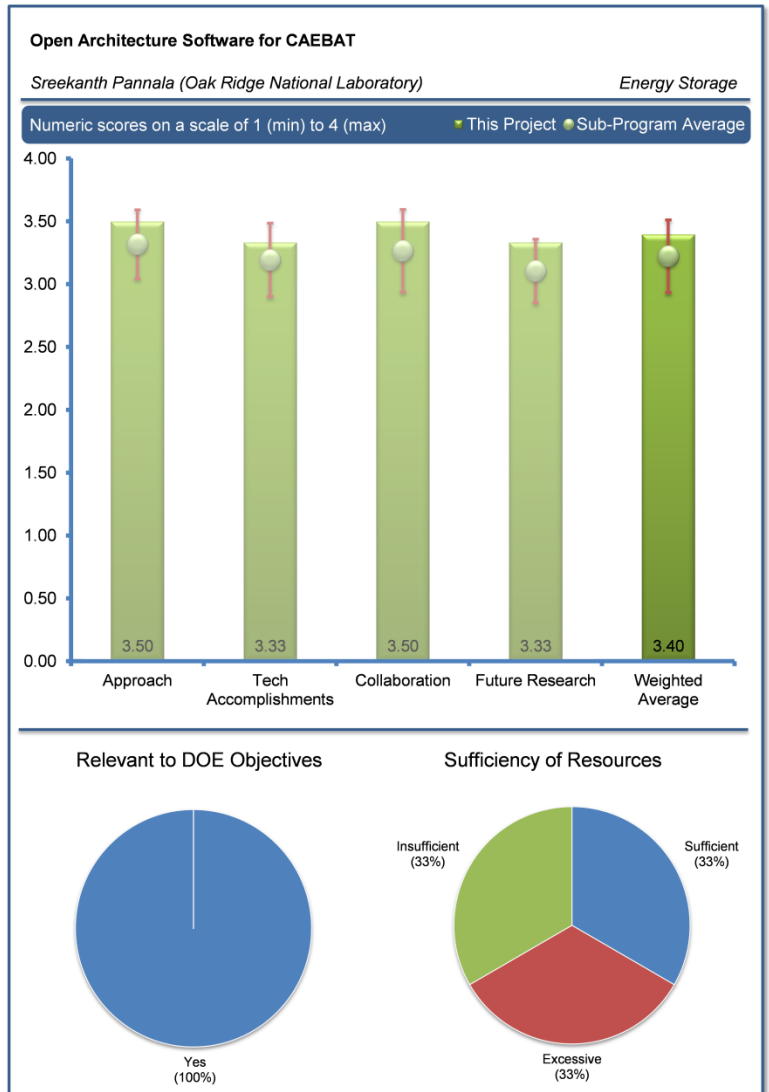
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

This reviewer commented the project for its well-executed and focused to goal achievement including scalability, standardization, and usability.

The reviewer noted thorough coupling and interfaces to build to larger devices (modules/packs).

The reviewer commented that the definition of the BatML as a “standardized” mark-up language was intriguing.



Reviewer 2:

According to this reviewer, this was a rather complicated, ambitious effort with its many components (OAS, VIBE, BatML, Battery State and NiCE). The indicated goal was a robust and user-friendly CAEBAT simulation platform. It was not clear how difficult this would be for users to learn and operate. The presentation does state that NiCE will permit users to easily switch components/choose from preconfigured inputs and that BatML may be edited through a standard XML editor. The reviewer added that the interactive (visual) component for these was an excellent feature. There was no indication of how well the project had succeeded in achieving its goals and what problems remained—without this information, the reviewer said it was difficult to judge what progress had been made. Perhaps some of this will only be determined through the use of the integrated software over time. It seemed that numerous presentations had been made regarding the outcomes from the project, but few written documents had been produced to demonstrate the capabilities of the work achieved. The reviewer asked if this software would ultimately only be for battery manufacturer and OEM usage (perhaps due to a high user cost) or if feedback from the integration of the models would also become widely available to battery researchers by some means.

Reviewer 3:

This reviewer said there were no solid accomplishment examples on integration of models. One example showing OAS to couple (or integrate) electrochemical (durafoil) and thermal components can be accomplished with the ECPower ECT model alone, said the reviewer.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

This reviewer noted that ORNL was the lead for this project. Collaborations are with NREL and the industrial partners (CD-adapso, EC Power and GM-Ansys teams). Other collaborations/coordination are with SNL (modeling capabilities), University of Michigan (modeling capabilities), Ford Motor Company and others. The reviewer concluded that the presentation suggests that this was a well-coordinated program with plenty of discourse and inputs from interested parties.

Reviewer 2:

This reviewer thought that there seemed to be good collaboration with specific roles described for each team member but that the collaborated integration results were not articulated clearly.

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.

Reviewer 1:

This reviewer noted that the ongoing milestones included the demonstration of the coupling possible from combinations of components from different project partners and the release/documentation of the User Environment V1 Software.

Reviewer 2:

The project will be completed by September 2014, said the reviewer, and agreed with the future research using the remaining fund.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This reviewer commented that the program to develop computer-aided design (CAD) tools for transportation batteries is well founded. Much of the technology and design developments for transportation batteries have matured and CAD tools will likely be the key to improving future designs and cost reductions for manufacturing. The reviewer continued to say that the work may also provide additional insight into fundamental science needs for battery materials. The reviewer concluded that the Open Architecture Software for this particular project seems to be the core, critical component for the integration of the different models developed as part of CAEBAT.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

According to the reviewer, no information was provided about the resources available, but it was assumed that these were sufficient.

Reviewer 2:

This reviewer pointed out that \$700,000 per year seemed excessive for integration effort. Some of the resources should be used to benchmark various battery models.

Development of High Energy Density Lithium-Sulfur Cells: Donghai Wang (Pennsylvania State University) - es125

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer simply stated that a solid and well-explained approach was being used.

Reviewer 2:

The reviewer applauded that the PI was taking an excellent approach to tackling the problem of identifying a higher energy density system than today's Li-ion system. The reviewer explained that the investigator planned to develop a full Li-S battery system which will include not only the nanocomposite sulfur cathode, but also the anode (Li or Si) and the electrolyte. The reviewer also noted that electrode dopants will be explored to prevent polysulfide dissolution. The reviewer also explained that the materials under investigation would be tested using 1.0 Ah pouch cells. This person stated this approach was far better than using coin cells since electrode performance does not always scale-up to a real manufactured cell. It was unclear to the reviewer how the team plans to investigate the mechanisms of polysulfide dissolution and self-discharge (Slide 10).

Reviewer 3:

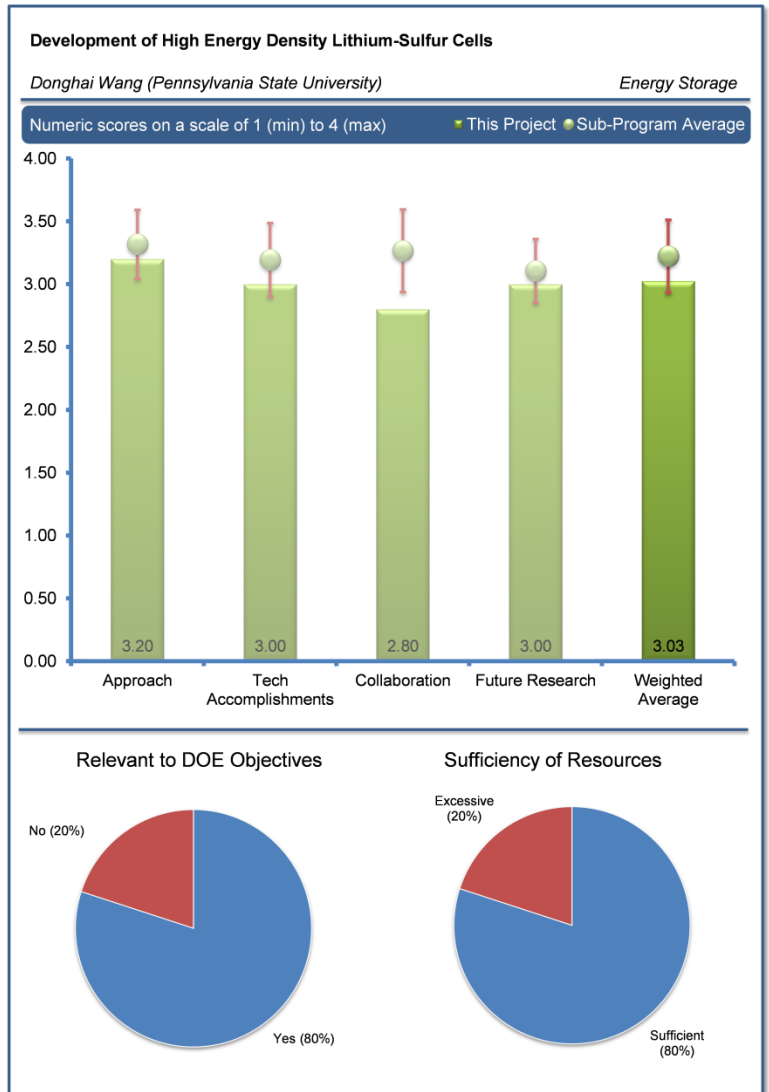
The reviewer reported that the project goal was to develop a lithium-sulfur (Li-S) metal battery system with a Li or Li-Si alloy anode for high current density, high energy storage capability and calendar life. The initial work concentrated on 1.0 Ah cells with potential for 600 Wh/l, cycle life of 500 cycles, and excellent safety characteristics. The reviewer noted that the researchers used a 1.0 Ah pouch cell as the experimental tool.

Reviewer 4:

The reviewer stated that although the researchers were using a comprehensive approach using the chemisorption materials, the project was still beset by all the well-known challenges of the Li anode. The reviewer also criticized that the goal of a 600 Wh/l energy density was too modest for such a large project when commercial Li-ion batteries are already hitting close to 800 Wh/l target.

Reviewer 5:

The reviewer agreed the approach seemed okay conceptually, but criticized that there was no detailed plan was offered that seemed likely to work. The reviewer noted that there was a lot of progress on durability, but power, and capacity are needed and the plan is not detailed. The reviewer exclaimed that without a plan that lead to the goal, the researchers will not get there. The reviewer reinforced that they did not hear a plan that was likely to meet the project goals when they talked to the presenter.



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.**Reviewer 1:**

The reviewer stated that the PSU-6 data looked impressive, but cautioned that the long-term and high temperature data were left wanting. The reviewer also asked what the N/P ratio is.

Reviewer 2:

The reviewer stated that this last year with a 1.0 Ah Li-sulfur (S) cell as a test vehicle, the properties reached over 400 Wh/l, scaled-up cathode to a 1.0 kg batch size and 600 and 500 cycles and good safety characteristics. The reviewer indicated that cycling testing was in progress, with 80% capacity retention results after 200 cycles. The reviewer also reported that a pressed carbon/sulfur cathode was developed with a 70% sulfur loading based on spherical phosphorous composite cathode with 70% sulfur loading; the cells had negligible self-discharge characteristic and good performance. This person also noted that cells with improved construction and LiNO₃ added gave stable cycle life for over 200 cycles with no degradation.

Reviewer 3:

The reviewer acknowledged that good progress had been made this past year. The reviewer explained that the investigators scaled-up their active materials to the 1.0 kg level and developed a 1.0 Ah prismatic cell with greater than 400 Wh/L that demonstrated 80% capacity retention in 200 cycles at the C/2 rate. The reviewer highlighted that it should be noted however, that the team must identify a system that is capable of more than 200 cycles. The reviewer pointed out that the PI's performance goal is 500+ cycles, so there is a long way to go.

Reviewer 4:

The reviewer recognized that the researchers have improved their cells in many ways, but asserted that the cells were still not to the level of commercial products. So, the reviewer said that good progress was made, but there was still a long way to go.

Reviewer 5:

The reviewer criticized that the prospects for achieving a viable cycle life in full cells did not appear to be promising.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer acknowledged that the PI had assembled an excellent team of research collaborators.

Reviewer 2:

The reviewer explained that the investigators were working with ANL on electrolyte development and on a Li powder based anode development for improved performance. The reviewer also stated that an independent evaluation of cells was being carried out at the INL.

Reviewer 3:

The reviewer expressed that there are good collaboration with other organizations that can provide support to this effort exists. The reviewer also mentioned that the researchers are partnering with EC Power. The reviewer explained that large-format Li-ion batteries are essential for vehicle use and EC Power can provide the expertise of transitioning any new materials developed into a viable battery. The reviewer specified that this effort would also benefit from the collaboration with ANL where concurrent electrolyte development is underway. This person said there is hope that, between the two laboratories, progress can be made to mitigate the poor cell performance.

Reviewer 4:

The reviewer proposed that partnership with at least one industrial partner might be beneficial to the commercial focus of project.

Reviewer 5:

The reviewer observed that the ANL collaboration was modest and that EC Power cannot give any real insight on production as they are effectively an intellectual property company and not an industrial firm.

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.

Reviewer 1:

The reviewer agreed that the proposed future work as outline on Slide 35 was reasonable.

Reviewer 2:

The reviewer explained that the future work will continue to work to scale-up both the anode and cathode in a prismatic configuration and optimize performance. Electrolyte development and stopping polysulfide migration will continue to improve performance will also be addressed. The reviewer reported that the cell size will be increased and safety testing will be carried out to define the cell's safety performance, as well a means to stop/slow polysulfide migration.

Reviewer 3:

The reviewer stated that the high temperature stability of the cell needs to be studied. The reviewer also asked whether the issue of battery management system development for this strange open-circuit voltage curve has ever been discussed; adding that must be a big challenge.

Reviewer 4:

The reviewer criticized that more detail was needed and recognition of the imminent end of the project merited a clear timeline which was totally absent in the presentation, but a discussion afterwards with the presenter revealed that a plan of sorts is present. The reviewer reported that at present the plan still included Li negative electrodes. The reviewer suggested that achieving the high current durability was probably a bigger problem that the researchers seemed to be ready for. The reviewer also suggested that some validation work in this area would be a good idea.

Reviewer 5:

The reviewer criticized that the scope of the extensive safety tests that are planned are unclear. The reviewer recommended that complete mechanical abuse testing, including crush be performed to demonstrate relative response of technology.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed that Li-S cells operating at room temperature and in a prismatic format should have superior energy storage capability. The reviewer also stated that their energy density and safety should be superior to most other Li cells.

Reviewer 2:

The reviewer stated that the project was highly-relevant to the goals of the DOE EERE, VTO (i.e., increasing specific energy from 100 Wh/kg to 250 Wh/kg and energy density from 200 Wh/L to 400 Wh/L).

Reviewer 3:

The reviewer agreed that Li-S systems, if made to work, would enable many DOE goals for electrified vehicles.

Reviewer 4:

The reviewer did not see this project as having any realistic chance of being deployed for vehicular applications; too many challenges.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that the resources were adequate for the planned development. The reviewer explained that continued success should lead to a new system that could have significant uses other than transportation.

Reviewer 2:

The reviewer highlighted that this effort was significant, and as a consequence, the total cost of the project was over \$5 MM. The reviewer reported that the amount of resources provided for this project appeared to be sufficient, which was evident by the amount of work that had been completed.

Reviewer 3:

The reviewer thought the funding level was too much for a project which has a long history of serious challenges.

Silicon Nanostructure-based Technology for Next Generation Energy Storage: Ionel Stefan (Amprius) - es126

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer's main concern for this technology for vehicular applications was whether it could be scaled-up cost-effectively, manufactured, and still beat the Wh/l value achievable using a conventional graphite electrode.

Reviewer 2:

The reviewer reported that silicon nanowire anodes had the capability to significantly improve energy storage capability. The reviewer also pointed out that the work should apply to other Li battery anode systems and cathodes for a breakthrough to double the present energy storage capability. The reviewer also mentioned that the anode physical structure is key for high-performance.

Reviewer 3:

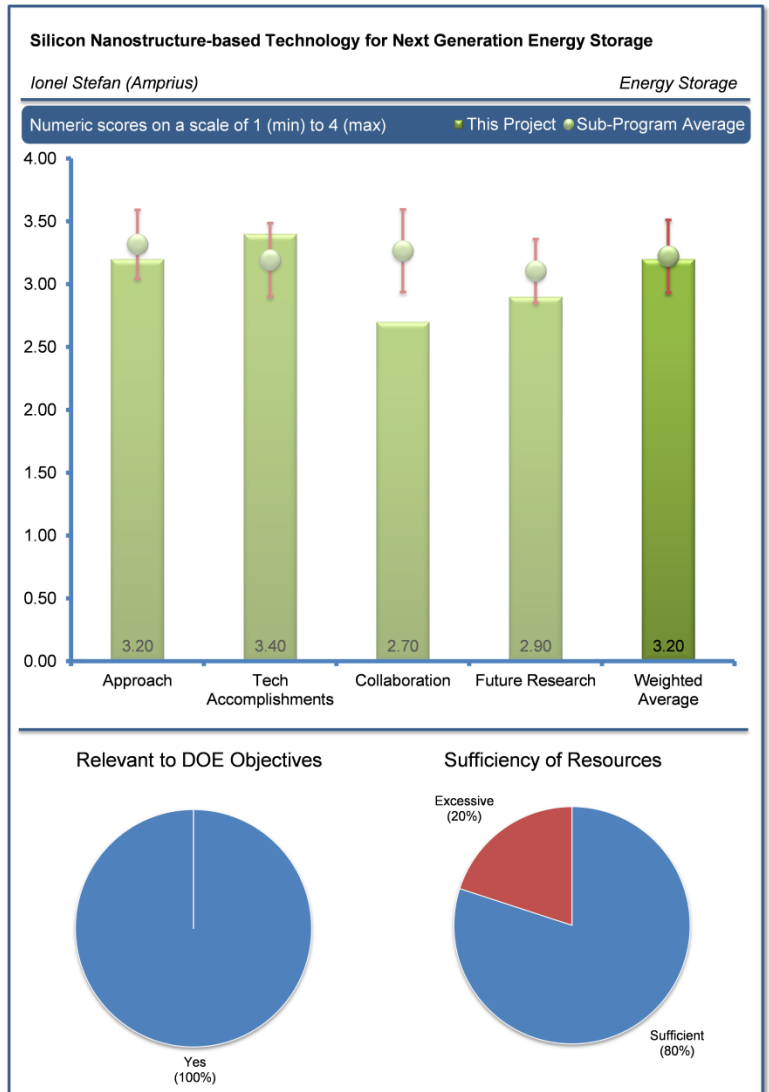
The reviewer said that it was nice to see a gated timeline and making progress to the planned trajectory. The reviewer agreed that Si nanowire directly attacks a key Si problem of swell fracture. The reviewer also noted that it was good to see the Hybrid Pulse Power Characterization test, an accepted industrial test, not some homemade test, be used for verification.

Reviewer 4:

The reviewer indicated that the approach was generally good or excellent in terms of technical demonstration, but appeared to have avoided investigation into, or explanation regarding, the potential costs related to manufacturing of this technology.

Reviewer 5:

The reviewer remarked that it was difficult to fully assess the approach that was being taken on this project. The reviewer asked what exactly was being done to meet the program goals other than developing growth-rooted silicon nanowires. The reviewer also wondered if there was a rationale for selecting certain electrolyte formulations and additives. The reviewer also requested if any information could be provided without compromising intellectual property.



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.**Reviewer 1:**

The reviewer stated that although good progress had been made, the results certainly were not the state-of-the-art. Even with conventional anode and cathode technologies, current consumer batteries are already in the 270 Wh/kg and approximately 785 Wh/l.

Reviewer 2:

The reviewer reported that Amprius had delivered 18 cells for testing at INL to confirm their findings. The cells were rated at over 700 Wh/l and 285 Wh/kg with a cycle life of over 500 cycles at 80% DOD. The reviewer noted that the anode construction should lead to good high rate performance as well as high energy storage capability.

Reviewer 3:

The reviewer could not find a presenter to answer some questions after the presentation, but thought there seemed to be good progress. The reviewer stated that it was nice to see durability only claimed to 80% (330 cycles and 700 cycles in early slides) and the progress is good and on trajectory. The reviewer wondered, while the deviation in cells sent for analysis was good, if there were many sorted out prior to sending off a hand-picked few, or do the results represent the true mean.

Reviewer 4:

The reviewer applauded that excellent progress had been made on this effort. The reviewer specified that an energy density of greater than 700 Wh/L and a specific energy over 285 Wh/Kg at the C/2 rate were achieved along with a cycle life of greater than 500 cycles.

Reviewer 5:

The reviewer commented that the project was a solid demonstration of significant energy density advancement with non-catastrophic cycle life in small format cell.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer noted that there was good collaboration among the key players in these technologies.

Reviewer 2:

The reviewer observed that there had been good cooperation with others developing Li anode cells. The reviewer also pointed out that national laboratories had been involved in independent cell testing.

Reviewer 3:

The reviewer would have liked to see domestic partners. The reviewer noted that Amprius was engaging the USABC, so should use those contacts to get more domestic advice and input.

Reviewer 4:

The reviewer explained that the majority of this effort was being conducted by the PI's company. This person noted that lower level effort was being conducted by BASF (cathode development) and Nissan (cell design). This was satisfactory if the PI wanted to maintain tight control of the project but may not be the most expedient method to advance the technology. Consultation with electrolyte experts would have been beneficial.

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.

Reviewer 1:

The reviewer expressed that the future plans were in keeping with the excellent opportunity to improve energy storage capability. The reviewer also indicated that the unique form of the anode was especially interesting.

Reviewer 2:

The reviewer indicated that this project was near its completion (ends September 2014). The reviewer reported that the proposed work was good, detailing that the researchers planned to complete the model of high volume anode manufacturing processes then deliver the 18 cells and final report.

Reviewer 3:

The reviewer reported that this was a well-funded project entailing cutting-edge anode and cathode materials. However, the reviewer cautioned that completion of the remaining work would not push the limits on scaling-up, manufacturing, or even energy densities. The reviewer recommended that the team focus on those aspects more than on refining a cell that was not state-of-the-art.

Reviewer 4:

The reviewer agreed that the future plans included the correct things to do, but criticized that the plans were vague on how this would be done.

Reviewer 5:

The reviewer noted that the project was nearly complete and that no future work plans were noted. The reviewer proposed that evaluation of basic relative abuse tolerance of technology in full cells, even on a small scale, would be beneficial.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer asserted that increased support should be in order as this was an outstanding development.

Reviewer 2:

The reviewer stated that, if successful, it would greatly raise the driving range of EVs.

Reviewer 3:

The reviewer explained that Si had emerged as one of the most promising next-generation anode materials for Li-ion batteries due to its high theoretical capacity. Unfortunately, the extreme volume change leads to rapid capacity fading; this effort addresses this problem.

Reviewer 4:

The reviewer asserted that this project definitely supports overall DOE objectives.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer remarked that sufficient resources were provided for this effort.

Reviewer 2:

The reviewer pointed out that while resources are adequate for the present program, an increase in resources should speed the development of the Li-alloy anode with exceptional performance.

Reviewer 3:

The reviewer agreed that there was more than enough cash, but also a decent cost-share level. The reviewer suggested that the PI needed to engage future customers in the battery industry and end-user customers much more aggressively.

Development of Large Format Lithium Ion Cells with Higher Energy Density: Fabio Albano (XALT Energy) - es127

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer observed that the project goal is to produce a large format prismatic cell with an energy density greater than 500 Wh/L and a cycle life of over 1,000 cycles to 80% of original capacity. The reviewer stated that, based on the results, the approach has been very successful. The reviewer also described that the program plan has been carried out in smaller cells, and in November 2014, the research team planned to produce large format cells for delivery to national laboratories for evaluation.

Reviewer 2:

The reviewer agreed that the development of large format Li-in battery was important. The reviewer said that the authors have shown progress; however, it was not very clear from where they are getting the advanced materials, and how reproducible the quality of such a material is.

Reviewer 3:

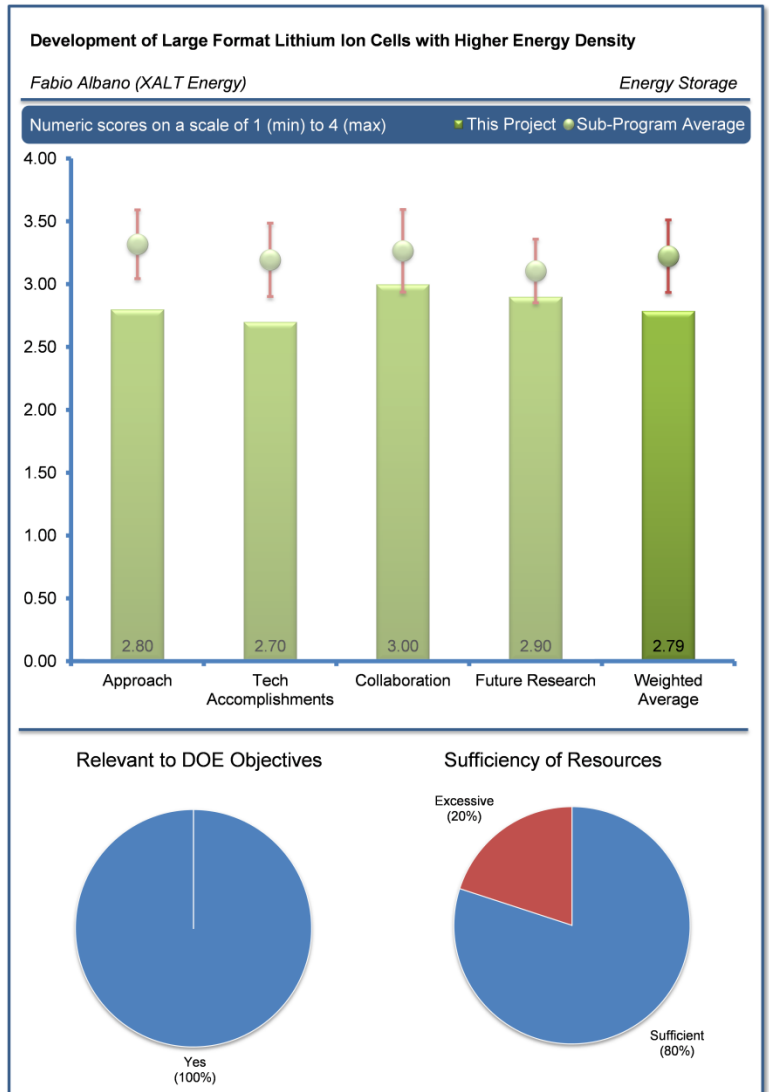
The reviewer summarized that the goal of this effort is to develop and demonstrate a large format Li-ion cell with an energy density of greater than 500 Wh/L and a power density of greater than 500 W/L. The reviewer pointed out that in order to meet these goals, new materials are required. The reviewer said that Wildcat Discovery Technologies is screening new materials and that there has been significant progress in this area which should be able to benefit the program. Unfortunately, it appeared to this reviewer that, from Slide 32, the cells continue to gas. The reviewer also noted that there is capacity fade (Slide 29). The reviewer had concerns that Wildcat Discovery Technologies may not be able to identify suitable materials within the time allocated for this project.

Reviewer 4:

The reviewer stated that the core-shell approach is nice, but asked what the rest of the system is; so, it was hard for this person to say if the approach is right without really knowing what the project team was working on.

Reviewer 5:

The reviewer stated that the project approach seemed to partially duplicate other funded projects.



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.**Reviewer 1:**

The reviewer stated that, based on differential scanning calorimetry curves of cells at ANL, the cells show excellent safety characteristics. The reviewer reported that the cell performance exceeds the DOE standard of 500 Wh/L. Nail penetration testing is next. The reviewer highlighted that the group had established a good track record of accomplishment.

Reviewer 2:

The reviewer cautioned that the authors should be careful about the specification of the raw materials that are proposed to be used in the future. The reviewer warned that these experimental powders were not easy to reproduce, in particular if they were under development.

Reviewer 3:

The reviewer stated that the progress seemed to be well behind the expected timeline. This person stated that the accomplishments are okay, but until durability and performance is seen it is hard to validate claims.

Reviewer 4:

The reviewer criticized that the progress made this year did not appear to be commensurate with the funding provided. The reviewer explained that many of the slides presented this year were the same as last year. For example, the accomplishments (Slide 20) looked almost identical to that submitted last year (Slide 13). Another example is that the cathode Slide 26 has a figure that is the same as last year's Slide 9.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer said that good collaboration existed within the project. The reviewer recounted that the team includes Wildcat Discoveries Technologies (Bin Li), ORNL (David Wood), ANL (Ira Bloom), NREL (G.H. Kim and A. Pesaran), University of Missouri, Kansas City (Xiaobo Chen), and the Department of Defense (Dilip Punatar).

Reviewer 2:

The reviewer indicated that the partners include Wildcat Discovery Technologies, the NREL, ANL, ORNL, and the University of Missouri, Kansas City for analytical work.

Reviewer 3:

The reviewer agreed that the extent of collaboration seemed reasonable in the case of XALT Energy's current technological maturity. However, the reviewer suggested that involvement of significant industrial partners would have the potential to greatly improve project focus and tangibility of project, even with reduced number of non-industrial research partners.

Reviewer 4:

The reviewer noted that there were lots of collaborators, but asked what their roles were. The reviewer said that other than NREL, the other collaborators were not mentioned. The reviewer also stated that ANL tested the researchers' cells, but that was a service that DOE provides so it was not really collaboration.

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.**Reviewer 1:**

The reviewer explained that in the future, the cell size will be scaled-up to 2.0 Ah. Increased cathode capacity will be considered as well as lowering the fabrication cell costs.

Reviewer 2:

The reviewer noted that the mitigation strategies are going to be critical.

Reviewer 3:

The reviewer commented that the future research was in the right direction, but that details were scant.

Reviewer 4:

The reviewer stated that the future efforts are satisfactory; describing that the work will continue on identifying high-voltage/high-capacity cathode materials. The reviewer also noted that a cost and biasness analysis will be conducted.

Reviewer 5:

The reviewer indicated that the plan for comparative abuse tolerance testing in large format cells or otherwise in any other full cells was not clear, but would be beneficial to project relevance.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer agreed that the project is very relevant, resulting in higher energy storage capability and potentially lower cost.

Reviewer 2:

The reviewer remarked that if the researchers succeed, the number of electric miles driven would go up.

Reviewer 3:

The reviewer reported that this project is relevant to DOE's goal as it is aimed at the development of an affordable, high-energy density battery.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that the resources are adequate for the present plans, but proposed that an increase is needed to meet the promise proposed.

Reviewer 2:

The reviewer said that it appears that the performer has sufficient resources to complete the work.

Modular Process Equipment for Low Cost Manufacturing of High Capacity Prismatic Li-Ion Cell Alloy Anodes: Sergey Lopatin (Applied Materials) - es128

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer affirmed that the approach taken is excellent; describing that it concentrates on methods to achieve a low-cost, high-energy density battery that includes investigating a new class of Li battery anodes and an innovative micro-porous 3D copper-Li alloy structure. The reviewer anticipated that the 3D electrode concept will increase capacity, fast charge capability, and result in improved energy and power densities.

Reviewer 2:

The reviewer reported that the prototype prismatic cell assembly line has been designed, constructed, and operated and the test cells based on NMC cathode and graphite (CuSbFe/Gr) alloy anode are being evaluated for their performance at INL. A new 3D CuSn anode is also under development. No detail was presented on the equipment or the design concepts. The reviewer said that it obviously works, but it is impossible to compare the cell assembly line with existing equipment.

Reviewer 3:

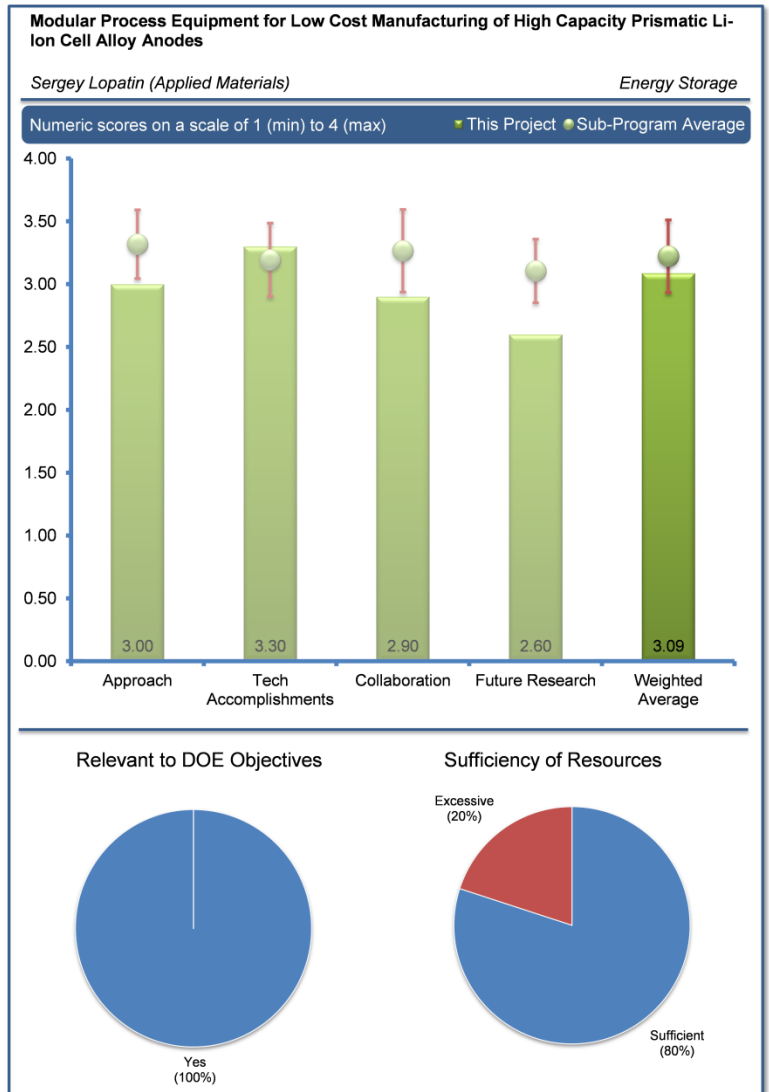
The reviewer highlighted that the approach was pushing boundaries in the right directions, but the reviewer would have liked the researchers to have better data that this could be done at low cost and quick enough to make millions of units per year.

Reviewer 4:

The reviewer claimed that the approach was excellent, or outstanding, in most technical respects, but appeared to avoid the understanding of, or focus on, the potential cost issues of this novel approach or its competitive manufacturing viability.

Reviewer 5:

The reviewer stated that the researchers have done some good work in looking at the impact of both rate and low temperature on the performance of their anodes. The reviewer added that the researchers also are cognizant of the importance of being able to wind their materials for roll-to-roll processing etc. The reviewer suggested that it would also maybe give them an earlier entry to the market if this technology could be applied to commercial Li-ion cells for the consumer market that use a wound construction. Fundamentally, the reviewer indicated that they do have a concern with the anode structure; the nanostructures deposited onto the substrate look to be very sharp and likely to cause internal shorting in real cells. The reviewer acknowledged that the researchers have apparently overcome this



by having a thick overlayer of carbon. The reviewer feared that if this layer is thick enough to protect the separator from the porous copper network, that the performance of that overlayer will not be any better than that of a normal Li-ion anode. The reviewer reported that the researchers' approach seems to excel in anchoring a thin layer of carbon or other anode material to the collector. The reviewer remarked that if a thick carbon overlayer is required either to get better capacity/area or to prevent shorting, it would seem that one would lose, at least in part, the benefits of their anode structure at the current collector interface.

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.

Reviewer 1:

The reviewer indicated that the researchers claimed good cycle life now and good capacity.

Reviewer 2:

The reviewer commented that excellent progress was made this past year. The reviewer summarized that Applied Materials completed the baseline cell characterization and the researchers developed a 3D CuSnFe nano-structure alloy anode that decreased electrode thickness and showed improved coulombic efficiency. During this process the reviewer reported that the researchers developed a water-soluble process for graphite coating and demonstrated high rate performance.

Reviewer 3:

The reviewer applauded the researchers' excellent progress and accomplishments to date in demonstrating the technical capability of the novel approach.

Reviewer 4:

The reviewer reported that the cell assembly line was designed and constructed and test cells were supplied for evaluation. The reviewer devalued the accomplishments, as no comparison with existing cell assembly equipment was included in the presentation. The reviewer concluded by asking why this concept was better.

Reviewer 5:

The reviewer explained that the researchers have shown that they can create effective anode/carbon structures. The reviewer also reported that the researchers have attained a significant increase in anode capacity, while still keeping the discharge potential of the anode low (so a full cell voltage will be high). The reviewer noted that the rate performance, low temperature, and cycle life look good. The researchers have also submitted full cells to DOE laboratories for testing, but no results are yet available. The reviewer would have liked to have seen some more fundamental work with the national laboratories. It seemed to the reviewer that the work by Wheeler et al., where they measure the bulk anode layer resistance and the interface resistance with the carrier, could be used to demonstrate and better understand the true benefits of this approach (Project Number es220).

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the team was excellent and included ORNL, LBNL, FMC, Navitas, and the Nissan Technical Center North America.

Reviewer 2:

The reviewer stated that this is mainly an industrial collaboration project. The reviewer would have liked to have seen some more fundamental work done with the national laboratory (e.g., modeling work to evaluate effect on conductivity/diffusion of their porous Cu layer with a thick graphite overlayer and collaboration with Project Number es220).

Reviewer 3:

The reviewer indicated that it was not clear whether the partners were having influence or if they were more than just contractors. The reviewer would like to see wider and more domestic input from customers in the battery industry and end-users in the automotive or consumer electronics industries so that they get the real picture of what is needed.

Reviewer 4:

The reviewer explained that there was no mention of outside collaboration, except for the test cells at INL. The reviewer also stated that evidently everything about the equipment is confidential.

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.

Reviewer 1:

The reviewer reported that the development of a new anode concept would continue. The reviewer cautioned that there was little detail, only reports of cell with copper anode current collector.

Reviewer 2:

The reviewer agreed that the future plans are good and will benefit the project. The reviewer explained that the cell will be manufactured and sent for characterization and analysis to LBNL and ORNL, who will characterize grain size, porosity and other parameters. Applied Materials, Navitas, and Nissan Technical Center North America will perform work on increasing the anode loading which will be demonstrated in battery unit.

Reviewer 3:

The reviewer explained that the anodes were fairly flexible, but it was not yet clear if they really could be wound at production speeds in a roll-to-roll manufacturing system. Thus, the reviewer highlighted that this was an important area that the researchers have identified as their next steps. The reviewer emphasized that the researchers needed to really follow-up on DOE lab testing to see how their anodes performed in real cells and also, with diligent analysis of the testing, provide some insight as to where to go next with this anode approach. This person pointed out that the researchers' plans to incorporate Si was also very important, although their plans involved a simple Si/C mixture and the reviewer was not sure if that would work very well. The reviewer commented that other people's approach of using Si with nano-tailored structures seems to be more promising from a technical viewpoint (although many of those other approaches may be unrealistic from a cost point of view), so the reviewer was not optimistic that their Si/C anodes will cycle well.

Reviewer 4:

The reviewer proposed that plans to evaluate the relative abuse tolerance response of the technology, even at a small scale, would be beneficial.

Reviewer 5:

The reviewer warned that the researchers were desperately behind their plan and that there was no recognition of this in the future work.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed that the project would indeed help meet DOE's goals.

Reviewer 2:

The reviewer asserted that this project is highly-relevant and supports DOE's objectives to displace petroleum with electric drive systems. For example, the EV Everywhere battery goals for 2022 are a cost of \$125/kWh and energy densities of 400 Wh/L and 250 Wh/kg. Reaching these goals will require significant improvements in material development and advanced high volume manufacturing.

Reviewer 3:

The reviewer commented that the project promises a substantial, albeit not revolutionary, boost to anode usable capacity, especially at high rate and/or low temperature. Thus, the reviewer indicated that the project could become really influential if the researchers could get it to work with Si, but the likelihood of success in this seemed low to the reviewer.

Reviewer 4:

The reviewer commented that the availability of cell assembly equipment with superior performance is needed; however it was impossible for the reviewer to judge the performance of the equipment itself from the presentation.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that the resources were adequate.

Reviewer 2:

The reviewer agreed that it appeared that sufficient resources were provided, as evident by the good progress that was made this past year.

Reviewer 3:

The reviewer cautioned that there was no need to spend dollars on demonstrating high-volume manufacturing (HVM) with this technique until a more firm background for the manufacturing costs associated with the process are demonstrated on paper relative to conventional processes.

High-Voltage Solid Polymer Batteries for Electric Drive Vehicles: Hany Eitouni (Seeo) - es129

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer described that the approach is to use a new approach to improve cell performance using a solid electrolyte that is non-flammable and non-volatile. The reviewer explained that this presents a significant opportunity to modify the internal construction of the Li-ion battery system with increased safety in operation, while still having the high energy advantage of the Li-ion cell system. The reviewer highlighted that the interaction with Hydro-Québec and their cell fabrication capability is a key part of the development.

Reviewer 2:

The reviewer commented that the approach taken during this effort was satisfactory; explaining that in order to achieve higher energy densities, a battery consisting of a Li foil anode is being developed. To do this however, the liquid electrolyte will be replaced with a dry polymer electrolyte binder/separator. The reviewer noted that having thin layers should enable good rate performance; however there are concerns that the polymer material being developed will not have the necessary electrode stability to reach DOE's cycle life goals.

Reviewer 3:

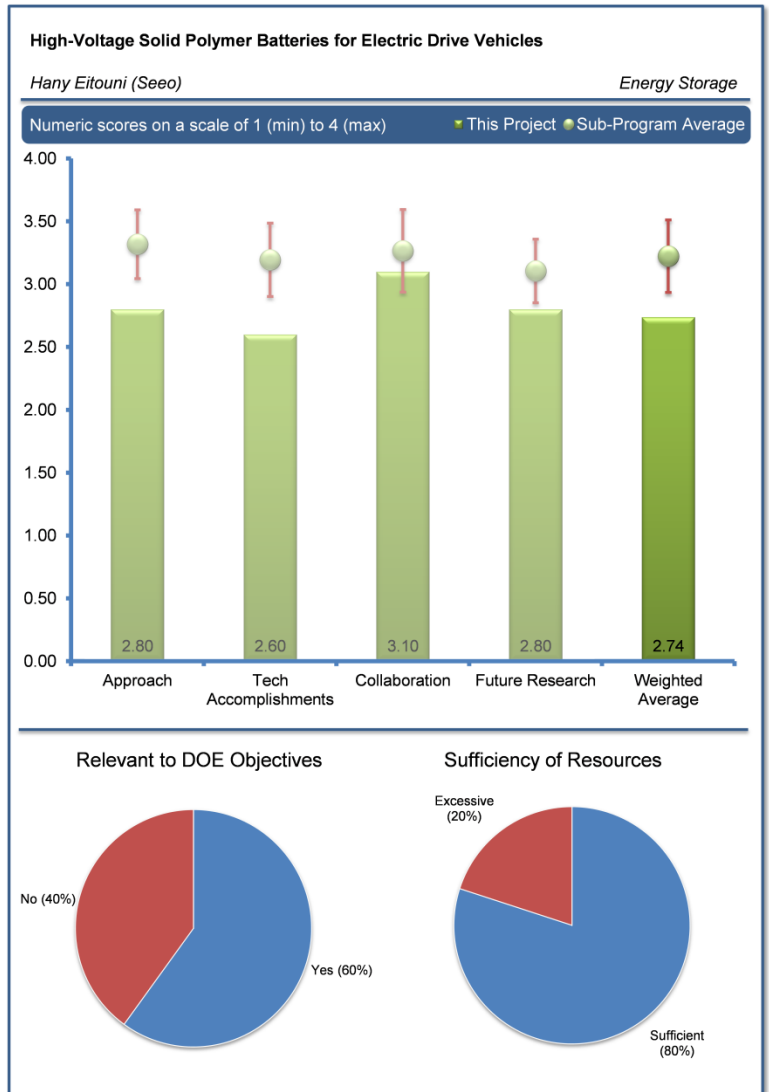
The reviewer acknowledged that the project uses an innovative solution, but pointed out that really hard questions about the cold weather use and parasitic power loss may just not be tolerated. The reviewer recounted that at least the researchers claim there is no permanent damage if it "freezes."

Reviewer 4:

The reviewer cautioned that the fundamental limitation of polymer electrolyte conductivity will limit the usefulness of this system for vehicular applications; however the reviewer added that it will find niche applications if developed successfully. This person indicated that multiple coatings were not the preferred routes for building a cost-effective battery. The reviewer also mentioned that coatings, if not conformal, are oftentimes band-aids, so might not meet the life targets.

Reviewer 5:

The reviewer criticized that the approach appeared to avoid performing work to address several of the fundamental issues with this particular technology. The reviewer explained that the scope of planned safety testing was unknown, but should be a key aspect of the project.



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.**Reviewer 1:**

The reviewer stated that work with Li anodes is challenging and hence the cycling results are not unexpected. The reviewer was not sure results better than these can be expected using the systems being studied in this project.

Reviewer 2:

The reviewer reported that Seo has developed a proprietary polymer electrolyte that is stable with Li anode materials. The reviewer added that the experimental cells were constructed and had excellent performance and cycle life.

Reviewer 3:

The reviewer reported that the interim cells were delivered to DOE this year. Numerous cathode coatings were evaluated and several have shown improved cycling performance in comparison to the uncoated cathodes. The reviewer stated that the cycle life was unfortunately limited as shown by Slides 10-12 of the presentation.

Reviewer 4:

The reviewer warned that 100 cycles is not nearly high enough and the project is nearing completion. The reviewer did note that it was good to see the timeline being held in other ways. The reviewer pointed out that the researchers said they have met 350 Wh/kg, though this was not very clear in the data so it was hard to be certain of the claim's accuracy. The reviewer reinforced that safety is still an issue, but indicated that the researchers seemed confident they can lick it.

Reviewer 5:

The reviewer criticized that the data shared in the presentation was offered in a form which allowed for little, to no, judgment of the technical accomplishments or progress.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer lauded that the collaboration with Hydro-Québec is a very positive situation. Hydro-Québec has full capability in cell R&D to carry out cell development and create a commercial product. The reviewer emphasized that this collaboration is essential for Phase 3 of the project.

Reviewer 2:

The reviewer applauded that teaming up with Hydro-Québec was a good idea.

Reviewer 3:

The reviewer confirmed that Hydro-Québec's participation in the project is a positive aspect.

Reviewer 4:

The reviewer asserted that the partners seemed to be interactive, which was not very common.

Reviewer 5:

The reviewer noted that Hydro-Québec is a collaborator and will provide support in the Li anode development, cell deliverables, and commercialization plan. It was unfortunate to this person that others with expertise in polymers were not included.

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.

Reviewer 1:

The reviewer explained that the third phase of the project involves the scale-up of material synthesis and design and construction of large area cells to validate the technology as well as develop a cell assembly process. The reviewer also reported that a cost structure will be developed to understand the cost of high volume production as well as the safety and cost issues for the technology.

Reviewer 2:

The reviewer simply stated that the future research was just what they need to work on.

Reviewer 3:

The reviewer agreed that the future planned efforts were appropriate for this stage of the program. The reviewer also stated that the final cell design would be tested and a commercial plan would be made.

Reviewer 4:

The reviewer proposed that there was no need to go to large area cells. The reviewer also pointed out that the safety testing scope was unknown, but was critical for demonstrating any future viability.

Reviewer 5:

The reviewer did not expect the researchers to solve the fundamental issues that were associated with this system; noting the high-temperature application and low cycle-life of the Li anode.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer confirmed that this project was highly-relevant to DOE's objective of petroleum displacement.

Reviewer 2:

In this reviewer's opinion, this was the most promising project at the Annual Merit Review. The reviewer remarked that cells with the Seo polymer electrolyte should have superior safety over the regular liquid electrolyte constructions and very similar charge-discharge capability.

Reviewer 3:

The reviewer stated that this work was one of the more "far out" stuff that DOE should fund, and yet it was very well along in maturity so that it could go to pack testing if a few bugs are worked out.

Reviewer 4:

The reviewer expected that only limited/niche applications would result.

Reviewer 5:

The reviewer proposed that due to the fundamental aspects and limitations of the technology, the project basis should be on stationary applications, or other non-DOE VTO applications, so it was not relevant for DOE VTO funding.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer emphasized that this project, above all others, deserves an increase in funding. The reviewer stated that present funding is adequate to demonstrate the capability, but a fast-track to commercialization will give the U.S. Li-ion community an advantage in safety while having equivalent performance to the regular Li-ion cells.

Reviewer 2:

The reviewer agreed that yes, the cash and the human resources seemed to be right.

Reviewer 3:

The reviewer simply stated that the funding appeared to be appropriate for this effort.

Innovative Cell Materials and Designs for 300 Mile Range EVs: Yimin Zhu (Nanosys) - es130

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer remarked that the advantage of scale-up/manufacturability of the SiN-anode made it an attractive system to study.

Reviewer 2:

The reviewer applauded that the development of the 1D silicon anode structure for Li-ion cells is excellent. The reviewer noted that using high capacity silicon will increase the energy storage capability, while the long cycle life of the experimental cells gives hope for a significant increase in cell capacity.

Reviewer 3:

The reviewer praised that the approach being taken in this effort was clearly stated and was in agreement with DOE goals. The reviewer explained that the investigators were tackling such problems as cell energy density and cycle life. A silicon nanowire carbon composite anode would be employed and results thus far looked promising to this person.

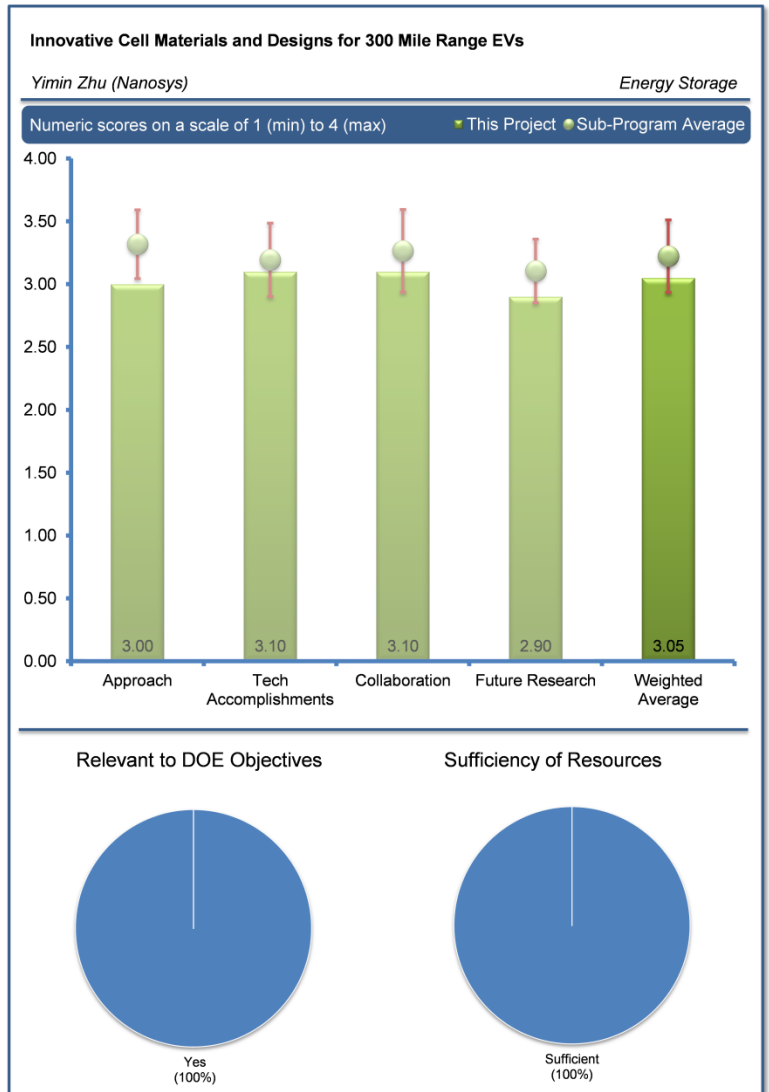
Reviewer 4:

The reviewer agreed that the basic approach was reasonable. The reviewer explained that the project is aimed at developing a Si wire carbon nanocomposite electrode whereby the Si lies on top of the carbon. The reviewer stated that the researchers' approach may overcome some of the physical damage that comes from carbon coating silicon particles, where the carbon coating can break up as the silicon expands during charge. However, the reviewer cautioned that with their approach of using Si on top of a carbon base, that the Si is always exposed to the electrolyte which might well lead to poor anode cycling as the Si gets used up in continual SEI breakdown and reformation with continued cycling. The reviewer also noted that the researchers looked at rate and low temperature performance, which was good.

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.

Reviewer 1:

The reviewer commented that the development of a Si anode with good performance resulted in an anode with excellent capability for long cycle life and high rate performance. The reviewer remarked that the Si anode has the capability to deliver up to 1,600 mAh/g



specific capacity. The reviewer also recognized that the cells have very low self-discharge on storage and a new electrolyte has been developed.

Reviewer 2:

The reviewer acknowledged that good progress was made this past year including a cylindrical full cell (SiN-anode/NCA) that had an 82% capacity retention at the 1,000th cycle. This cell was also shown to have a higher anode capacity than the graphite anode containing cell.

Reviewer 3:

The reviewer stated this was a scalable method that uses little, or no, gold. The reviewer remarked that the concept shows decent packing, so was likely okay on a volume basis as well. The reviewer emphasized that this was important, as some of the elegant methods people have developed fall down in this area. The reviewer also simply noted that good cycling data was presented.

Reviewer 4:

The reviewer observed that the key challenge of long cycle-life still remained a formidable one. The project person also noted that cells achieving an energy density of 550-700 Wh/L were already a commercial reality using conventional anode and cathode technologies.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer indicated that the researchers were working with key developers, who could give good feedback on the direction of work.

Reviewer 2:

The reviewer summarized that the project had interacted with A123, LG CPI, Dow Kokam, Farasis Energy, as well as several national laboratories.

Reviewer 3:

The reviewer stated that the researchers have made good choices and involved industrial partners.

Reviewer 4:

The reviewer praised that the team, including A123, LG CPI, LGC, Dow Kokam, Farasis Energy, and several of the U.S. DOE laboratories, was very good. It was unclear to the reviewer what the role was of each of the various laboratories shown on Slide 23.

Reviewer 5:

The reviewer stated that this was mostly an industrial partnering program. The reviewer did not see much sign of integration with, or leveraging of, experts in DOE national laboratories. The reviewer asked whether this approach should not also be included in the cell builds and testing being done at ANL.

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.**Reviewer 1:**

The reviewer described that the plans were to scale-up the cell fabrication to optimize cell performance, develop additives to improve electrolyte performance, improve cycle life and cell design.

Reviewer 2:

The reviewer agreed that the future work being proposed was appropriate. The reviewer described that the focus would be on improving the cycle life of the anode, including optimizing the cell by minimizing the inactive components, improving the cell design, and optimizing the cathode material composition. The reviewer also mentioned that it was good that cell evaluations at low temperatures are being conducted.

Reviewer 3:

The reviewer expressed that the researchers needed to focus on high loading, or at least high enough for a power-based HEV cell (ideally work on a PHEV design that uses a thicker electrode would also be carried out). The reviewer offered that the researchers needed to ensure that the future testing includes some work with ANL to build and test the standardized cells so that their method can be compared to other approaches to using silicon anodes on an apples-to-apples basis.

Reviewer 4:

The reviewer stated that the project ended this year and that there were no indications of the researchers' intent for future work.

Reviewer 5:

It was not apparent to the reviewer how the key bottlenecks of low cycle-life, energy density, and cost targets would be met in future research.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer commented that since the concept was much more amenable to scale-up, and if the cyclability/cost issues could be resolved, then this project would be valuable to the overall goal.

Reviewer 2:

The reviewer stated that new high-performance Li-ion cells to power cars would reduce petroleum use.

Reviewer 3:

The reviewer asserted that this project was highly-relevant and supported DOE's objectives to displace petroleum with electric drive systems. For example, the EV Everywhere battery goals for 2022 are a cost of \$125/kWh and energy densities of 400 Wh/L and 250 Wh/kg. The reviewer explained that achieving this would require lowering the cost of raw materials and material processing, as well as lowering the cost of cell and module packaging and manufacturing.

Reviewer 4:

The reviewer confirmed that this work could lead to a better anode, but that it was hard to say whether it would be better than other Si/C anodes under development.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer agreed that the resources were adequate for the proposed work.

Reviewer 2:

The reviewer commented that based on the results thus far, the resources were sufficient.

High Energy Novel Cathode / Alloy Automotive Cell: Jagat Singh (3M) - es131

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer called the approach the right one, noting that the researchers are utilizing high-energy cathodes with new-generation anodes and tested on 18650 cells.

Reviewer 2:

The approach being taken in this project, the reviewer said, is clearly defined and a logical path toward meeting DOE goals and observed that the team plans to develop a high-performance cell using high energy-density and low-cost advanced electrochemistries. The reviewer went on to note that the cathode will utilize a core-shell design, the shell consisting of high Mn content for improved cycle life and a high Ni content for good capacity and that Si alloy anode is also being developed. These materials, the reviewer said, are known for their high capacity.

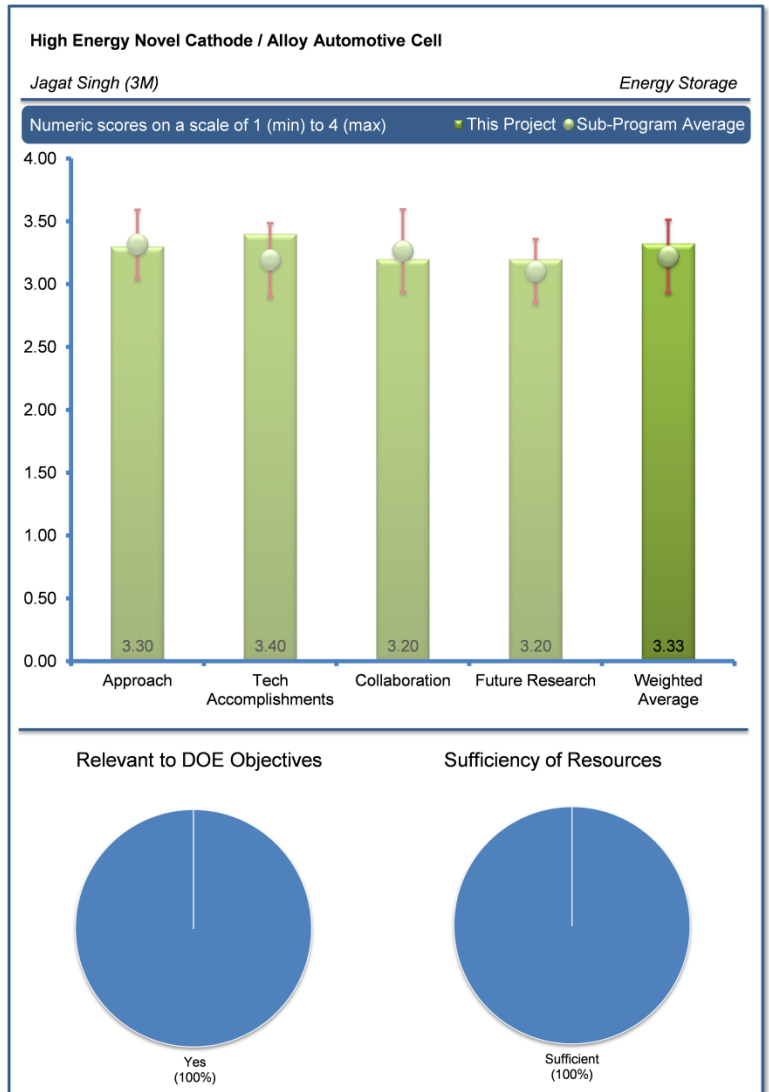
Reviewer 3:

The reviewer termed the approach solid, tangible and well-focused. An additional area which could have been or could be included (and beneficial), the reviewer suggested, would be limited comparison of abuse tolerance relative to baseline cell in 18650 form. Perhaps this is included in the project's thermal stability plan, but this is not clear, the reviewer said.

Reviewer 4:

The basic approach is reasonable, the reviewer felt, and aimed at marrying a high-capacity, core-shell NMC with silicon-carbon alloy. This, the reviewer said, could lead to a modest, but still useful advance in energy density. One advantage the reviewer saw for the project team's approach is that the electrodes are practical from a manufacturing point of view.

The reviewer would have liked to see some more fundamental work done on the chemistry of degradation with cycle life and/or basic electrochemistry. The reviewer explained that the team infers that cathode instability is causing the voltage fade at high states of charge. The reviewer called the cycling followed by half-cell cycling nice work and said it supports the team's belief. However, the reviewer would have liked to see much more use made of other electrochemical tools to better understand the cause of the problem, specifically, differential capacity plots and/or reference electrodes, which the reviewer said can be very helpful in fully understanding the causes of poor cycle life.



Reviewer 5:

The reviewer described the project goal as being the development of a battery for an electric vehicle with 40% greater energy density and 25% lower in cost over present systems and noted that high-performance silicon alloys for the anode and improved NMC performance are the key elements.

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.**Reviewer 1:**

Very good progress has been made this past year, the reviewer said, noting that the team developed electrode coating procedures and delivered baseline and intermediate cells. The NMC cathode scale up appears to be successful the reviewer observed, and the pilot plant material gave similar performance to the lab material. The reviewer also noted the development of a cost-effective process for commercially viable Si alloy anode materials, in addition to the evaluation of high-voltage electrolytes and demonstration of a 18650 format cell with a 40% energy improvement.

Reviewer 2:

The reviewer noted that the researchers mentioned having produced 100 kg. of advanced material (anode) and wondered how much (in kg.) had been produced per day. The core-shell concept seems to be working, the reviewer said, again asking how much could be produced per day and how reproducible the quality of such material was.

Reviewer 3:

The team were able to get higher capacity from anode and cathode, the reviewer observed, albeit with poor cycle life at full capacity. Reducing charge voltage so the cell is not fully charged helps a lot, the reviewer said, but noted that this is true even for commercial Li-ion cells. However, the reviewer said, the penalty in energy needed to attain good cycle life is quite substantial in this case. Overall, the reviewer felt, this does not represent much of an advance. The reviewer found it hard to discern the extent of the capacity loss from undercharging the cell from the normalized plots in the presentation.

Reviewer 4:

A new high-energy NMC cathode material was developed, the reviewer blandly noted, as well as new silicon anode structure with high performance. Fade on cycling also was reduced for long life, the reviewer said, and a 40% energy improvement was obtained along with a 40% improvement in cycle life.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer cited excellent and sharply focused collaboration without unnecessary distractions.

Reviewer 2:

The reviewer cited good interaction between ANL, Dalhousie University and 3M.

Reviewer 3:

The PI is teaming with Dalhousie University who has a superior background in lithium battery technology, the reviewer said, predicting the university will bring great value to the team. Likewise, the reviewer observed, Argonne National Laboratory is helping by improving testing procedures and providing valuable insight regarding the materials.

Reviewer 4:

Terming this a mainly industrial collaboration project, the reviewer felt the team could benefit from better collaboration with the national labs, especially their electrochemists and staff who have methods to study cathode fade.

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.

Reviewer 1:

The reviewer strongly encouraged the electrochemical testing on 18650 cells and predicted the thermal stability test is going to be important.

Reviewer 2:

This effort is scheduled to be completed January 2015, the reviewer noted, and for the remaining time, 18650 cells will be evaluated, the team will continue to develop and test electrolytes for improved cycle life and the thermal stability of the cells will be tested. These tasks are appropriate and will contribute to the development of a cell that comes closer to meeting DOE goals the reviewer stated.

Reviewer 3:

The reviewer expressed the hope that useful relative abuse tolerance comparison is included in thermal stability testing plans.

Reviewer 4:

Noting that the project team was focusing on a better electrolyte to get the cycle at higher voltage, the reviewer described this as a major project in itself. Acknowledging that the fluorinated electrolytes might work, the reviewer felt the likelihood of success or other significant trade-offs (rate capability) with them seem pretty high. This project team, in the view of this reviewer, was facing a major challenge and could benefit from more help and advice from the national laboratories.

Reviewer 5:

Proposed future work includes EV testing of the new NMC material with silicon anodes in a new electrolyte, establishing the thermal stability of the system and developing new electrolytes for Phase 3 of the project, the reviewer said.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

This project is relevant to DOE's objectives to displace petroleum with electric drive systems, the reviewer said. Obtaining affordable batteries will require lowering the cost of raw materials and material processing, as well as lowering the cost of cell and module packaging and manufacturing, the reviewer concluded.

Reviewer 2:

The project could enable higher energy density while using electrodes that are producible on a large scale, according to this reviewer.

Reviewer 3:

The new cells will have greater energy storage capability and longer life, the reviewer said.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

Sufficient resources are available, the reviewer said.

Reviewer 2:

In the opinion of this reviewer, the program appears to have the necessary resources to complete the tasks successfully; the total project funding includes \$4,577,909 (from DOE) and \$1,961,961 from the company.

Utilization of UV or EB Curing Technology to Significantly Reduce Costs and VOCs in the Manufacture of Lithium-Ion Battery Electrodes: Gary Voelker (Miltec UV International) - es132

Reviewer Sample Size

A total of two reviewers evaluated this project.

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.

Reviewer 1:

The approach appears attractive from the standpoints of solvent usage, cost, etc., in the opinion of the reviewer, who was less sure about long-term life data.

Reviewer 2:

The reviewer noted that the project is intended to show that UV-curable binder technology can be applied to Li-ion cells and said the process was clearly demonstrated on NMC material. The reviewer felt the process should be able to handle most metal-oxide-based cathodes. This advancement will contribute significantly in the reduction of capital and manufacturing costs associated with Li-ion cell fabrication, the reviewer predicted.

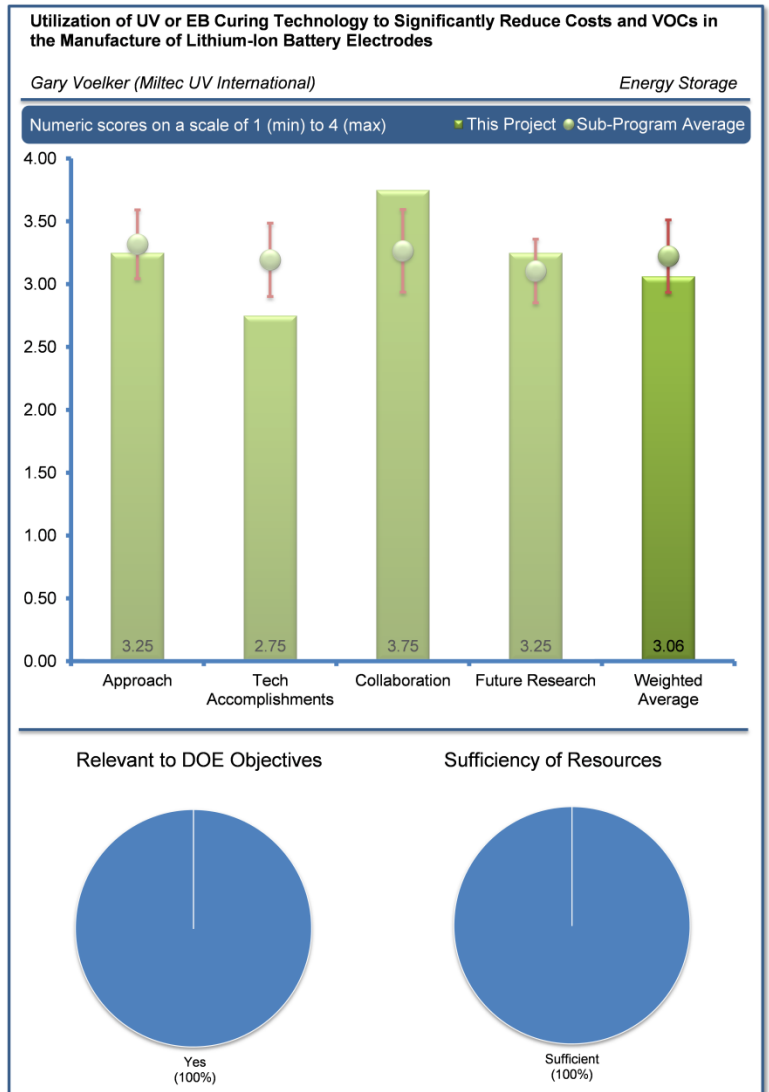
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

Observing that the data so far is quite preliminary, the reviewer expressed the concern that all the data are from half cells and that, even after three years, the project team have not been able to present data on full cells. Of course, the reviewer said, cycling of such cells at elevated temperatures will be a key test for the validity of this process.

Reviewer 2:

The reviewer felt the project has lacked in comprehensive performance analysis, but had achieved expected material density and cyclability. The anode work has taken longer than expected, the reviewer observed, but the investigator has learned about the issues associated with various electrode systems. The success with the separator work the reviewer deemed an additional bonus. The reviewer looked forward with interest to seeing the performance of a cell utilizing multiple fabricated components and encouraged the generation of a complete gap chart, summarizing initial project goals, and the degree to which these were achieved.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

There is good coordination with suppliers and testing labs, the reviewer said, which is ideal for the scope of the project.

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.**Reviewer 1:**

The reviewer recommended the project team devote efforts to fabricating and testing full cells to demonstrate the efficacy of this process and to then test the cells at elevated temperatures, too.

Reviewer 2:

The project is closing out, the reviewer noted and would benefit from further development with a larger-scale cell development partner. The reviewer encouraged such follow-on development.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

If validated, the reviewer stated, this process has the potential to significantly lower cell manufacturing cost.

Reviewer 2:

This project is an excellent example of improvement in manufacturing processes for advanced batteries, the reviewer said.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

Resources were well balanced for the project, which was capital intensive, with significant process development, the reviewer said.

Significant Cost Improvement of Li-Ion Cells through Non-NMP Electrode Coating, Direct Separator Coating, and Fast Formation Technologies: YK Son (Johnson Controls) - es133

Reviewer Sample Size

A total of two reviewers evaluated this project.

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.

Reviewer 1:

The approaches promise significant cost advantages, the reviewer said, and if the processes and performance are validated, will definitely help develop low-cost batteries.

Reviewer 2:

The reviewer termed this a multi-pronged approach to generating novel manufacturing processes for high-cost components, none of which was particularly innovative, but which were executed with a solid balance between cell design, performance, and manufacturability, in the opinion of the reviewer.

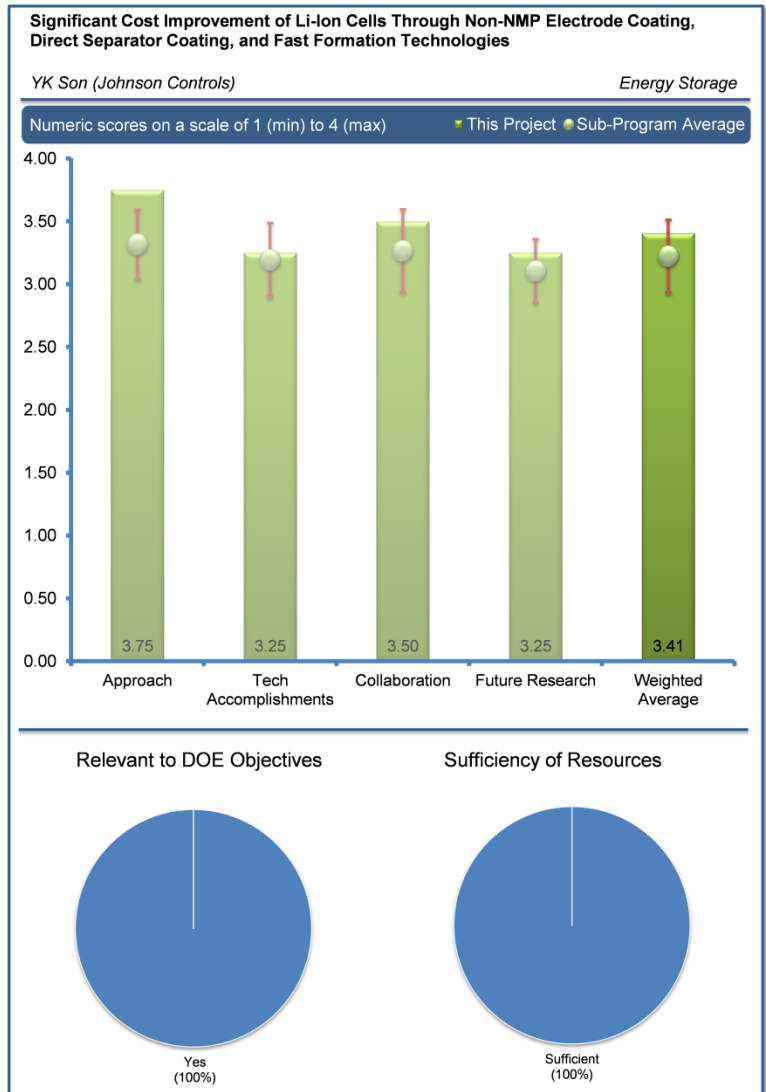
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The poor rate capability at continuous currents, the reviewer said, is a significant issue that needs to be addressed for these technologies to be potentially useful for Li ion battery production. The reviewer expressed the understanding that dry electrode manufacturing can be applied only to thick electrodes and it is a challenge for fabricating high-power, thin electrodes. The reviewer inquired about how the project team would address that.

Reviewer 2:

Overall, the reviewer found the results impressive. Among the results, the reviewer regarded the dry process electrode as particularly intriguing. The key targeted barrier was fabrication costs, the reviewer noted. The baseline cost indicated for process appeared to the reviewer to be very high, particularly when contrasted with the materials cost. This engendered a degree of skepticism in the reviewer concerning the true cost reduction over best-in-class cell manufacturing. The reviewer encouraged the inclusion of more cycling data and abuse results in future reports.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer regarded this as an excellent team for collaborative work.

Reviewer 2:

Noting that it was not explicitly stated which partners performed what portion of each of the tasks, on each slide, the reviewer nevertheless found it clear that solid coordination between the key partners occurred.

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.**Reviewer 1:**

The reviewer observed very good prioritization of future work, and expressed confidence that the results of this program will be transferred to production. The reviewer recommended the PI report the cost improvement in terms of \$/kWh for a representative cell design, in order to emphasize the savings.

Reviewer 2:

The reviewer recommended that validation of fabrication, power, life (at elevated temperatures) in the proposed 15 Ah cells, as well as cost modeling be the focus of future work.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The project is highly relevant, the reviewer said, since it targets the reduction of battery cost.

Reviewer 2:

This reviewer observed excellent demonstration of manufacturing improvements to reduce battery cost, which remains the single largest barrier to mass adoption of PEVs.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The project is well planned and executed, the reviewer said.

Dry Process Electrode Fabrication: Mike Wixom (Navitas Systems) - es134

Reviewer Sample Size

A total of two reviewers evaluated this project.

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.

Reviewer 1:

The reviewer said the approach to anode and cathode coating was multi-pronged.

Reviewer 2:

Listing the objectives of the project as developing dry process cathodes of suitable thickness to meet the rate and cycle life needs of EVs; identifying binder system for solvent-free anode fabrication stable through 500 cycles; validating the cost savings from the process improvements; and demonstrating the performance in prototype cells, the reviewer felt the approach to developing low-cost fabrication processes is valid, but also felt there should be no compromise in performance, since any performance reduction will indirectly impact the cost. Also, the reviewer said, the methods being developed are dependent on the active materials (in this case LFP and NMC cathodes).

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.

Reviewer 1:

Noting that there is some good progress relative to dry cathode and low/zero-solvent anode, the reviewer termed it encouraging. The NMC-LFP (50:50) blended, dry-processed cathode shows reasonable rate capability and comparable cycle life and impedance values as for the LFP cathode, the reviewer observed. Likewise, the reviewer noted that development of anodes from high-solids aqueous anode slurry with advanced drying process, or with dry blending alone, is showing some promise, but there are still issues related to cycle life. Referring to the comment of a previous reviewer, this expert agreed it is important to have proper standards (baseline) for comparison, both in terms of performance and cost. A realistic cost analysis, the present reviewer said, is required to justify the effort here.

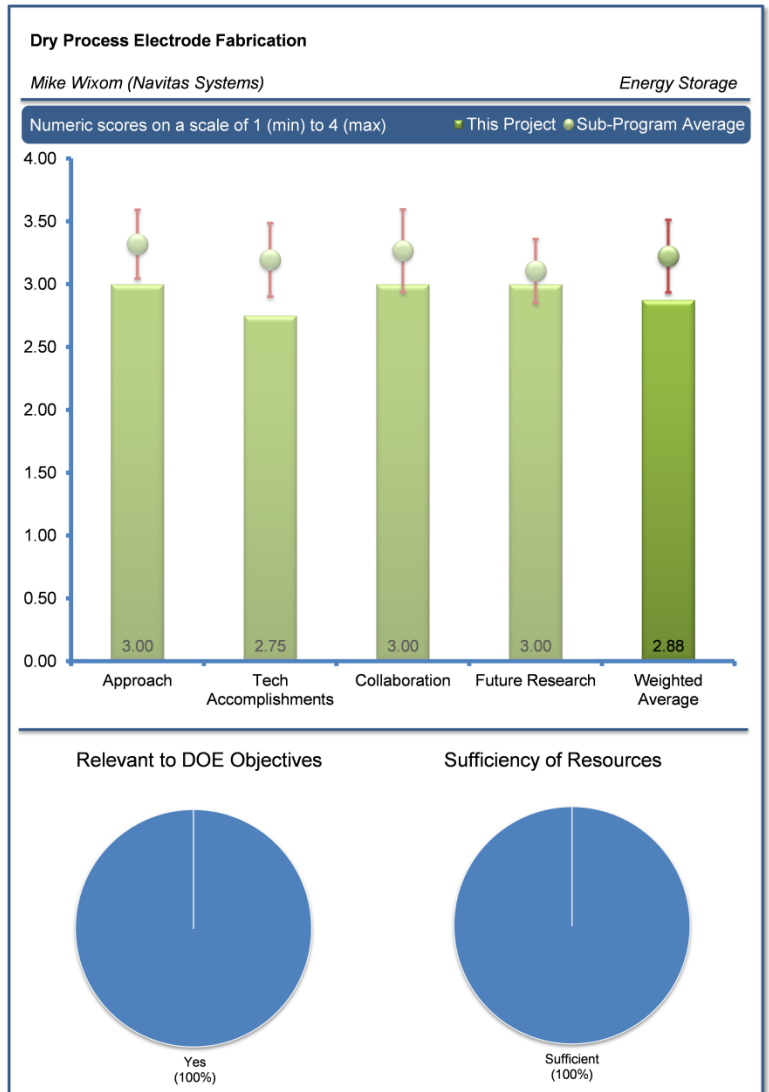
Reviewer 2:

Progress has been good, the reviewer said, although a more structured gap chart would help in evaluating the results. Calling the moisture issues with full cells a setback, the reviewer recommended including data from a baseline cell, utilizing traditional processes.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Saying there is no formal collaboration here, the reviewer noted a few ongoing, unfunded collaborations on various materials.



Reviewer 2:

The program is driven by Navitas, the reviewer said, with a supplier-customer relationship with most partners.

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.

Reviewer 1:

The reviewer deemed the plan solid, given both the original project plan, as well as response to discoveries and encouraged the PI to include details on electrode thickness and process performance, as indicated in the original program objectives.

Reviewer 2:

Citing the proposed future research as including identification of alternate processing additives for the cathode to mitigate moisture retention and increase active material content and to further improve calendaring to get wider cathode films; reformulation of dry anode to reduce initial capacity loss and down-select and scale-up anode process for final cells; and demonstration of the performance of low-cost process anode and cathode in full cells, the reviewer called these future plans consistent with the overall goals of the ABR program of reducing the cost of Li-ion cells. However, the reviewer went on, it is important to make a proper assessment of cost savings from this improved process, with assistance from a commercial EV battery manufacturer, if possible.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

High specific energy, long cycle life and low cost are the performance drivers for Li-ion batteries in electric vehicles, the reviewer stated. Cell fabrication processes for Li-ion cells are cost-intensive – as much as the cost of cell components, if not more, and this project, the reviewer said, is aimed at developing alternative low-cost cell (electrode) fabrication methods to lower the costs of Li-ion cells and increase their adoption in electric vehicles.

Reviewer 2:

Along with the future work, the reviewer said, this project will aid in reducing manufacturing costs for large-scale cells.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The resources are well-balanced, in this expert's view.

Reviewer 2:

The resources are adequate, in the reviewer's opinion, maybe even slightly excessive for the scope of the project.

Stand-alone Battery Thermal Management System: Brad Brodie (DENSO International America) - es135

Reviewer Sample Size

A total of one reviewer evaluated this project.

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.

Reviewer 1:

After establishing a suitable battery simulation model that could also incorporate thermal system modeling in Phase 1, the reviewer observed, subsequent efforts in Phases 2 and 3 focused on evaluating various thermal design concepts through modeling and validating the concepts down-selected through bench testing with a battery pack of high energy. Two thermal design concepts (reactive thermal management though high-efficiency vapor-compression cycles and passive thermal management) were also studied in detail and will be further explored with prototype samples of the selected technologies through bench testing, the reviewer concluded.

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.

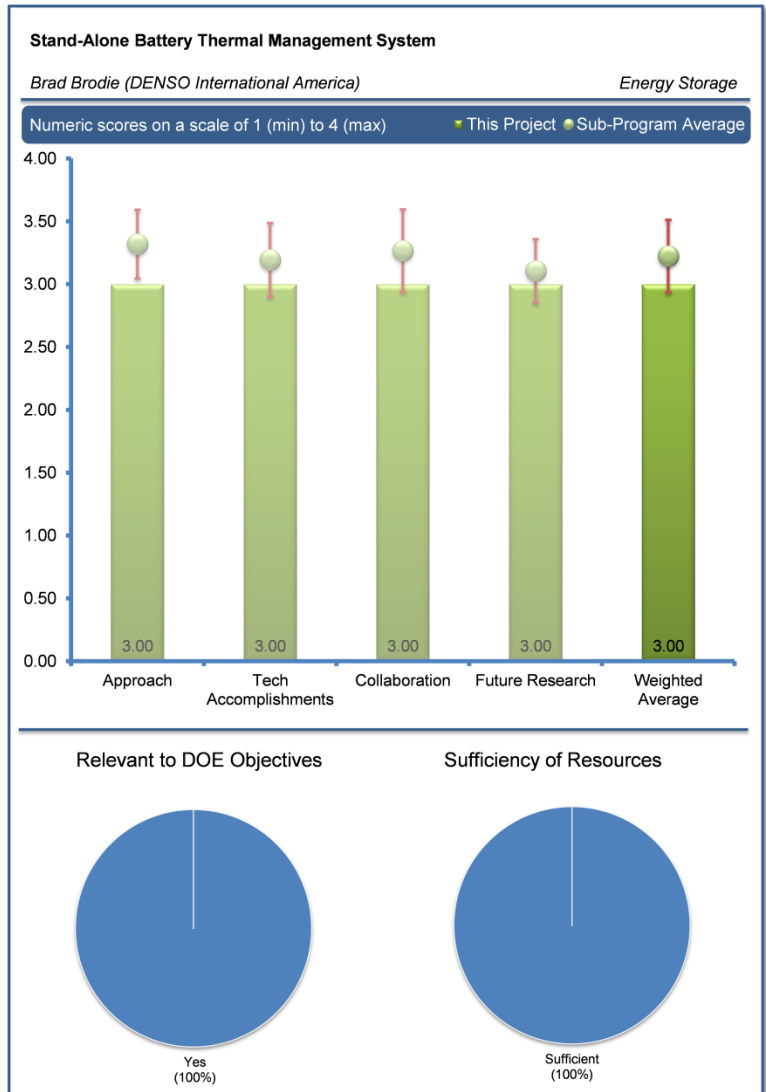
Reviewer 1:

Good progress has been made toward the project goals, the reviewer said, noting specifically the battery simulation model created in Phase 1 with NREL's help, and verified with the vehicle data from Chrysler. This model, the reviewer said, predicts battery life, fuel economy and energy effects of thermal system based on vehicle usage and ambient conditions, battery heat generation and the selected thermal system. These analyses show that a heat pump system is more efficient than resistive heating and can reduce battery-heating energy more than 50%, the reviewer observed. With aggressive thermal management, it is possible to increase the battery lifetime by 3 years in the worst climate, and reduce the battery active material by 5% (over 8 years). These predictions are useful engineering guidelines in the design of proper thermal management, the reviewer said, and need to be verified experimentally. One difficulty with this project the reviewer noted is the lack of adequate fidelity for the battery simulation model for performance and degradation (first-principles) due to its complexity and specificity for the battery chemistry.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

This is a good collaborative project with a national laboratory (NREL) and the EV user (Chrysler), in the opinion of this reviewer, who noted that NREL will further collaborate in the testing of the thermal management system and Chrysler will provide the battery pack.



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.

Reviewer 1:

Proposed future research, the reviewer said, will include subjecting prototype thermal system components to bench testing to validate and demonstrate the effectiveness of the thermal system, which will be done both at DENSO and NREL. These plans are consistent with the goals of the ABR program of reducing the size and cost and improving the life and safety of Li-ion batteries, in the reviewer's opinion. With the simulation tool developed here, the reviewer continued, it is probably useful to study other thermal management schemes currently being used in EV batteries for a comparative assessment of the cost and efficacy of the selected thermal management methods.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer cited high specific energy, long cycle life and low cost as the performance drivers for Li-ion batteries in electric vehicles. For Li-ion batteries, the reviewer stated, thermal management is crucial to ensure not only long cycle life and adequate safety, but high specific energy at the battery level and this project aims at developing innovative thermal management concepts that reduce the cell or battery weight, complexity (component count), and/or cost by at least 20%.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The resources are adequate, the reviewer said, perhaps even slightly excessive for the scope of the project.

Innovative Manufacturing and Materials for Low-Cost Lithium-Ion Batteries: Steve Carlson (Optodot Corporation) - es136

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

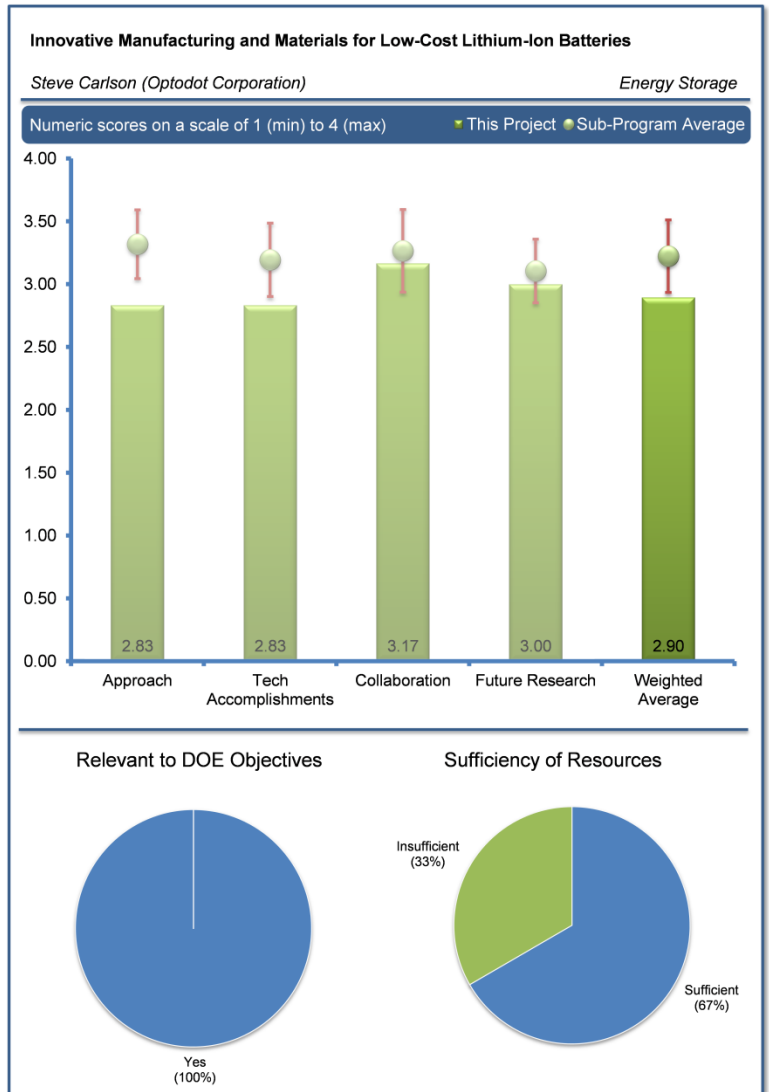
The technology shown, the reviewer said, is an excellent extension of prior art technologies, but directed specifically at the DOE objectives. These were clearly identified at the start of the presentation, and supported throughout, the reviewer continued, but some concerns exist over the magnitude of the project and degree of progress.

Reviewer 2:

The reviewer felt the approach adopted here appears to be viable and is consistent with the objectives of ABR. The approach is based on replacing the conventional polyolefin separators with thinner (8 micron) ceramic separators, the reviewer said, which, because of its dimensional stability, provides improved safety and high-temperature operation, and can enable new electrode production processes – coating the active materials directly onto the ceramic separators and using thinner current collectors. Overall, the reviewer said, there will be a 20% decrease in cost and more than a 5% reduction in volume. Consistent with the approach, proprietary processes have been developed to deposit thin current collectors onto the electrode later. In addition, new, non-flammable electrolytes are being developed, the reviewer noted, although not much detailed information was provided on this subject in the presentation. These improvements, the reviewer said, are being demonstrated in 2 Ah cells to show the feasibility of the concepts.

Reviewer 3:

Somehow, the reviewer stated, the targets set for this project (250 Wh/kg; 400 Wh/l) are not aligned with reality. Lithium-ion batteries offering approximately 270 Wh/kg and 780 Wh/l are a commercial reality in late 2014, the reviewer noted. The reviewer was left unsure what targets the project team is working toward. Nor was the reviewer sure that the cost reduction from thinner components (separators and foils) would not be outweighed by processing costs. How will the uniformity of the electrode/separator interfaces and that of the electrode porosity be controlled, the reviewer asked. The reviewer also wondered if the electrode stack will survive the typical pressure used to calendar electrodes.



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.**Reviewer 1:**

Overall the improvements appear promising, the reviewer said, and likely to reduce the cost and overall volume of Li-ion cells. The reviewer felt questions remained, however, namely, whether these ceramic separator-based electrode stacks are amenable to cylindrical cell designs and if there are apt to be any mechanically induced failures (from vibration and shock) of the ceramic separator. Good progress has been made toward the project goals, the reviewer went on, by demonstrating the thin current collector/active material/separator stacks with thin ceramic separators. Specific areas of progress included development of ceramic separator and release substrate to achieve defect-free electrode/separator stack coatings, which would further reduce the ceramic separator cost by about 20% and demonstration of good cycling at room temperature of initial prototype separator/electrode stack full coin cells with thin Al and Cu current collectors. In addition, the reviewer said, the cells with ceramic separators have shown good low-temperature performance and high-temperature stability.

Reviewer 2:

The program, as reported, appears to be running late, the reviewer observed, and significant work has yet to be achieved. The fabrication process has been demonstrated, but it will be good to see the results of the complete cells, the reviewer went on.

Reviewer 3:

The cycling data, being preliminary, shed very little light on the capability of such a cell fabrication process, in the opinion of this reviewer, thus long-term and high-temperature cycling are needed to validate the stability of such interfaces.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

A strong team for collaboration, the reviewer said.

Reviewer 2:

This, the reviewer said, is a good collaborative project, with participation by four partners and subcontractors – Madico, XALT Energy, URI and Ashland for different aspects, i.e., coating and converting expertise and equipment, battery assembly and testing capability, electrolyte expertise, and polymer and solvent expertise.

Reviewer 3:

It was not clear to this reviewer the degree to which the development partners have been engaged to date and the reviewer recommended the PI indicate partner engagement on the appropriate slides.

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.**Reviewer 1:**

The plans are consistent with the project goals, the reviewer said, and went on to describe them as including further optimization and scale-up of the anode and cathode stacks, the current collector/terminations; development of coated stack designs with one-third thinner electrodes for high rate/power cells; continued evaluation of new lithium salts and flame-retardant electrolytes; understanding the mechanism of enhanced cycle life with thin (8 micron) ceramic separators; assessing the cost savings with these improved cell designs and delivering cells for performance and safety demonstration.

Reviewer 2:

The reviewer expressed concern over the degree of technical work that will be required in developing internal tabbing, since this will form significant portion of development work, once the two-electrode cell construction is worked out. The reviewer encouraged the PI

to investigate an EV-representative design cell, as part of a paper study, in order to pro-rate performance cost, and assess manufacturing/scaling issues.

Reviewer 3:

Instead of diluting the efforts on new work such as nonflammable electrolytes etc., the reviewer felt, the project team should focus on validating the cell results by carrying out long-term cycling at high temperatures.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This process holds promise of significantly reduced cost, the reviewer said, and urged that the program be followed through with a more applied program to demonstrate scale-up.

Reviewer 2:

Efforts to improve process and lower component costs are important for developing low-cost batteries\for automotive applications, the reviewer stated.

Reviewer 3:

High specific energy, long cycle life and low cost are generally the performance drivers for Li-ion batteries to be used successfully in electric vehicles, the reviewer said. For the current Li-ion cells, the reviewer continued, performance is satisfactory, but the cost and weight are rather high and this project aims at reducing the overall cost, weight and volume of Li-ion cells by 20-40%, without affecting the performance, by reducing the cost, weight, and volume of inactive components (separator, electrolyte, current collectors)

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The resources are slightly excessive for the scope of the project, though the projected improvements are attractive, the reviewer said.

Reviewer 2:

The PI indicated that the project is approximately 50% complete, with three months remaining on the program timeline, the reviewer noted.

Novel Anode Materials: Jack Vaughey (Argonne National Laboratory) - es143

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

In the judgment of the reviewer, the approach aids understanding of the operation of Si-based anode and potential replacement of current lithium-ion batteries for increased energy density and safety.

Reviewer 2:

The reviewer noted that the investigators used a methodical approach to the study of Si anode SEI formation and said it will be interesting to see how the techniques utilized can be applied to the more complex composite anodes being proposed by industry.

Reviewer 3:

The approach is good, the reviewer said, and suggested that a comparison of electrodeposition and PVD could be made.

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.

Reviewer 1:

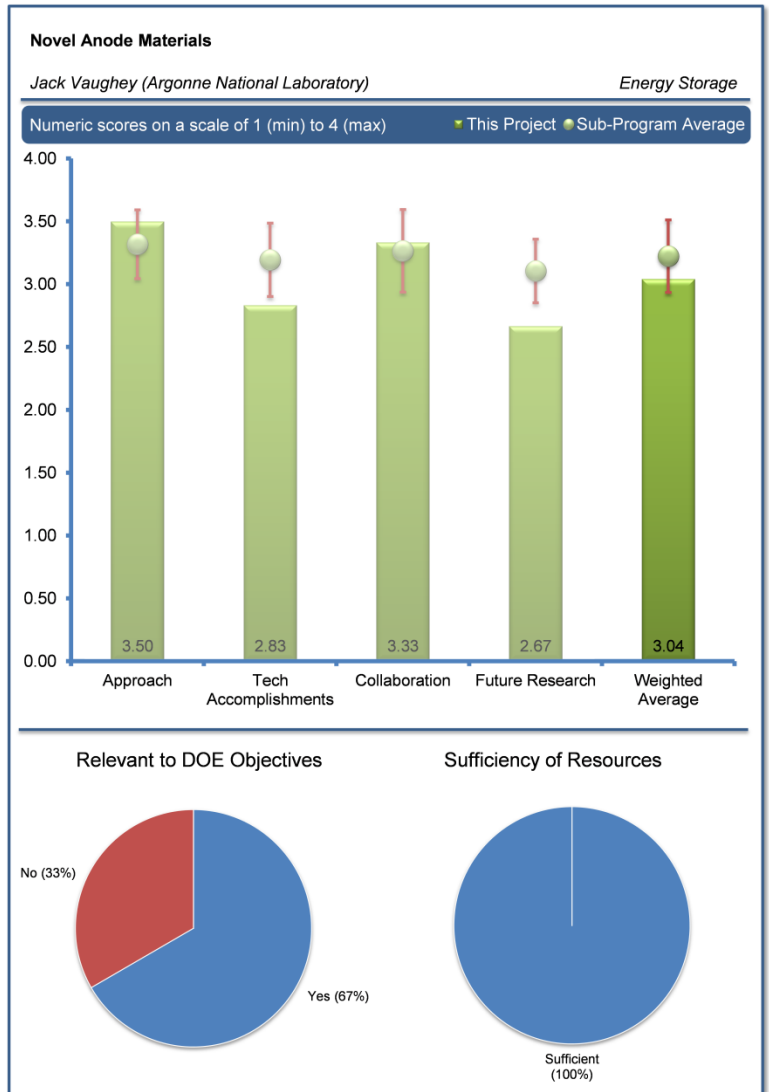
This project has achieved interesting results, the reviewer felt, but the cycling efficiencies are still relatively low and the first-cycle capacity loss appears to be high. The reviewer observed that the interface between SEI and Si appears to play one of the key roles for the Si-based anode and wondered what the relationship of that role is to the cycling rate.

Reviewer 2:

The research has made solid strides toward determining a core mechanism for an ionically conductive SEI layer, the reviewer said. The reviewer felt, however, that the work is more a research effort than an effort to develop a solution to the main problems cited in the introduction.

Reviewer 3:

The reviewer cited accomplishments including interfacial Cu₃Si formation and to improve the loading. However, the reviewer regarded most of the published papers listed as not relevant to the silicon work.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The PI has collaborated closely with other institutions, one reviewer said.

Reviewer 2:

Most work was done by the prime research facility, the reviewer stated, but the partners' results were clearly included within this report.

Reviewer 3:

Collaboration with other institutions is good, in the opinion of the reviewer.

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.**Reviewer 1:**

It may be helpful, the reviewer suggested, if work on the impact of the charge/discharge rate can be included to understand the degradation caused by lithium silicates.

Reviewer 2:

It was not clear to the reviewer whether the future work will achieve its goal in overcoming the barriers listed, namely, being able to engineer a stable, high ionic conductivity SEI layer for a Si composite electrode.

Reviewer 3:

The project team should describe the type of stable materials that may influence the degradation pathways, in the opinion of the reviewer.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer described the project as addressing the problems associated with Si-based anodes for improved Li-ion battery specific energy and safety.

Reviewer 2:

The reviewer felt the technology developed herein will be difficult to apply to anodes practical for plug-in EV batteries.

Reviewer 3:

Reduce the use of petroleum was stated by this reviewer.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

There are sufficient resources allocated for this project, the reviewer said.

Reviewer 2:

Progress appears reasonable, with respect to the current level of resourcing, this reviewer felt.

Reviewer 3:

Sufficient resources were observed by the reviewer.

Development of High Capacity Anode Materials: Jason Zhang (Pacific Northwest National Laboratory) - es144

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer said this project structure was impressively well focused, balancing a creative perspective on the problems, while remaining focused on the goals.

Reviewer 2:

This project, in the reviewer's judgment, addresses some key technical barriers of Si-based anodes, including Si expansion.

Reviewer 3:

Porous silicon approach is a very good idea, in this reviewer's opinion.

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.

Reviewer 1:

This project, the reviewer said, has achieved several progresses accomplishments, and electrode capacity retention can be as high as over 80% after 1000 cycles for certain electrode loadings. FEC additive has been proved to be effective for capacity retention, the reviewer noted, but found it unclear if the additive can be valid over a wide temperature range. The reviewer pointed out desirability of demonstrating capacity retention at a higher rate during cycling.

Reviewer 2:

Progress has been impressive, the reviewer said. The reviewer encouraged the investigators to continue to focus on scale-up to thicker electrodes, and begin the optimization of pre-lithiation, and to characterize electrode impedance and rate capability. Future work, the reviewer said, could then move to additional optimization for electrode rate performance.

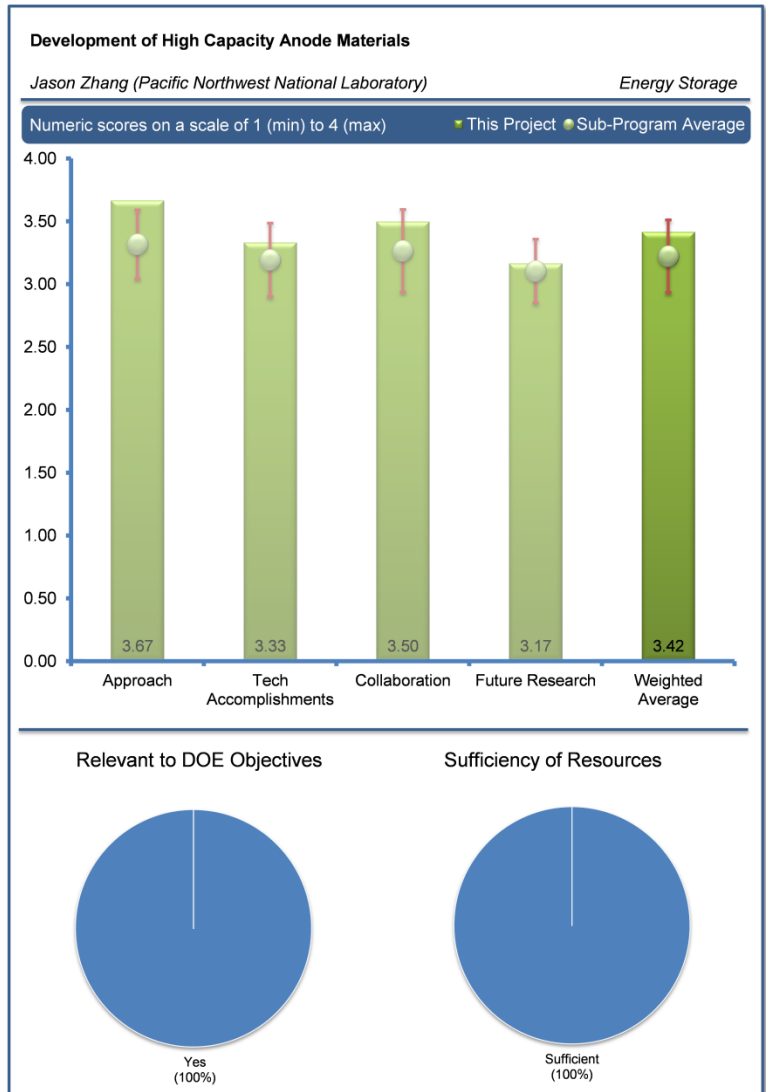
Reviewer 3:

This reviewer inquired about how to improve the loading and whether the prelithiated samples can be made stable in air.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The PI has a close collaboration with other institutions, the reviewer observed.



Reviewer 2:

The investigator clearly identified the collaborative roles and the collaborators contributed significantly to the overall program, in the view of this reviewer.

Reviewer 3:

Collaboration is very good, in the opinion of the reviewer.

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.

Reviewer 1:

The PI proposed several approaches to future work, the reviewer noted, but it was unclear to the reviewer if that future work could be accomplished under this project (which is to be ended by September 2014) or for a future project.

Reviewer 2:

The reviewer directed attention to earlier remarks but did not specify which ones. The investigator, the reviewer said, has laid a firm base for future work, and should be ready to begin to move towards a more application-based investigation.

Reviewer 3:

Noting that in the presentation summary it was indicated that low-cost electrodes have been developed, the reviewer pointed out that the future work also indicates low-cost electrodes will be developed. The reviewer questioned the nature of any cost difference between these groups of electrodes.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

This project, the reviewer said, supports the DOE objectives by targeting some key technical barriers of Si-anode capacity degradation.

Reviewer 2:

This technology should be transferable to practical cell designs, suitable for PEV applications, the reviewer stated.

Reviewer 3:

Reduces the use of petroleum was stated by this reviewer.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

There are sufficient resources allocated for this project, in the opinion of this reviewer.

Reviewer 2:

Discerning no issues, the reviewer cited good program management.

Reviewer 3:

There are sufficient resources allocated to this project, the reviewer said.

Atomic Layer Deposition for Stabilization of Amorphous Silicon Anodes: Chunmei Ban (National Renewable Energy Laboratory) - es145

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer called the program an excellent example of the application of novel scientific approaches to a practical problem. The project was executed with clear, targeted focus on the goals, and the approach uses lessons learned from previous activities in the battery field very effectively, the reviewer stated.

Reviewer 2:

The novel technical approach, the reviewer said, addresses some key barriers for Si-anode applications. Cost analysis may need to be considered for ALD and MLD approaches, the reviewer added.

Reviewer 3:

The ALD and MLD approaches are new, this reviewer said, but the cost has to be indicated.

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.

Reviewer 1:

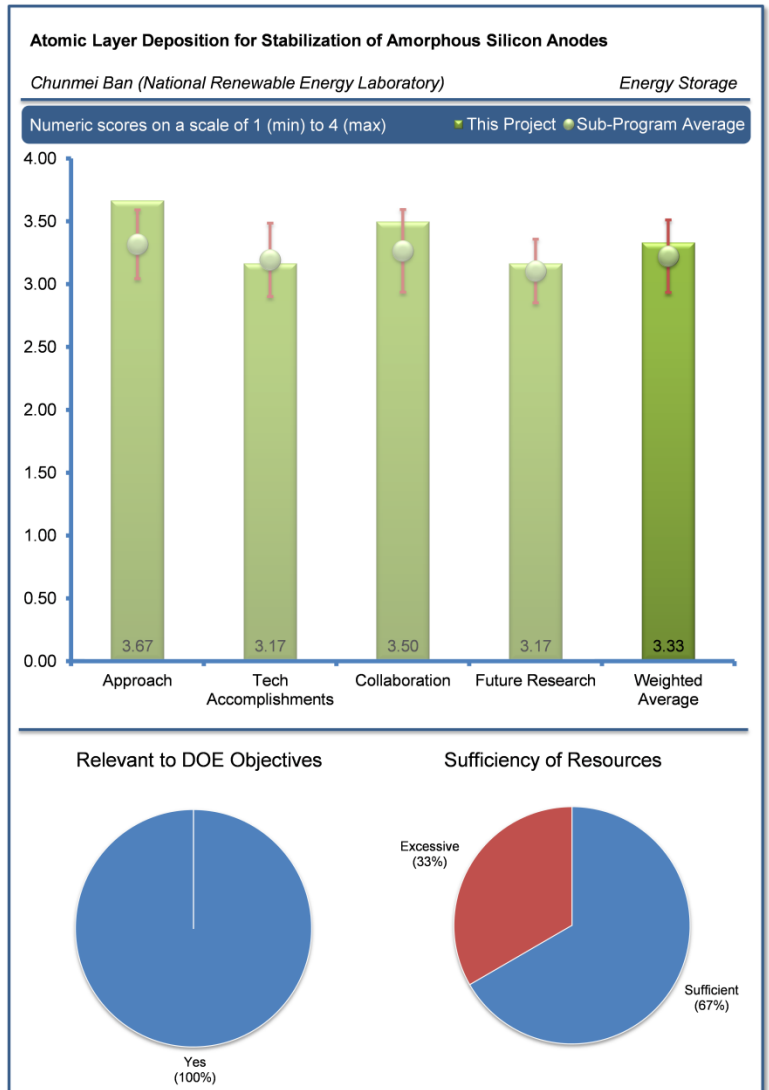
Accomplishments have been impressive, in the judgment of this reviewer, who noted the investigator’s indication that the project is complete, and the subsequent description of future work yet to be done. The reviewer professed support of the notion that additional work be done, but requested clarification of whether this is part of the current program, or a future program.

Reviewer 2:

This project appears to have achieved some interesting progress, the reviewer said, but more progress in capacity retention and charging efficiency during cycling are desired.

Reviewer 3:

The reviewer inquired about how to improve the loading using ALD and MLD. The reviewer noted indication that MLD alucone coating has been developed to significantly improve both energy and power capability for Si anodes. New coating conditions for ALD/MLD are being developed in order to coat electrodes more efficiently and work at atmospheric pressure, which will greatly reduce cost. The reviewer considered that the strategy for cost reduction was not clear, along with how the challenge of improving loading was to be met.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

In the judgment of this reviewer, the project has excellent collaboration with many institutions.

Reviewer 2:

The team was well organized and effectively utilized, in the opinion of the reviewer.

Reviewer 3:

The collaboration is good, the reviewer said.

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.**Reviewer 1:**

The proposed work is reasonable, said the reviewer, who offered the suggestion that pre-lithiation could help reduce the first efficiency issue.

Reviewer 2:

Future work was not detailed, since this program is closing, the reviewer observed, expressing a desire to see more investigation of this method with the use of binder systems considered more suitable for Si electrodes, in order to determine whether synergies between materials and methods can be exploited.

Reviewer 3:

An experimental approach describing how ALD and MLD are performed should be provided, along with cost reduction, the reviewer said.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The project addresses Si-anode capacity retention through coating for improved lithium ion battery energy density and life, the reviewer observed.

Reviewer 2:

This method, in the opinion of the reviewer, could potentially be implemented into the manufacture of Si electrodes.

Reviewer 3:

This reviewer said the project reduces the use of petroleum.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

There are sufficient resources allocated for this project, in the opinion of this reviewer.

Reviewer 2:

The team assembled was very large, given the work, the reviewer said, but conceded having no direct knowledge into how much time each team member assigned to this project.

Reviewer 3:

Project resources are sufficient, the reviewer said.

Synthesis and Characterization of Polymer-Coated Layered SiOx-Graphene Nanocomposite Anodes: Donghai Wang (Pennsylvania State University) - es147

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

This project, the reviewer said, is well-designed and targets both Si-anode (Si-C nano-composite) and binder to attack the battery cycle life and electrode kinetics.

Reviewer 2:

Calling the project an excellent example of applying innovative materials techniques to develop high-performance electrode components, the reviewer also noted that, like most of the associated research projects, there is an absence of cost analyses for the synthesis methods and resultant materials.

Reviewer 3:

The reviewer regarded approaches for development of silicon anodes as new and unique. Boron doping, the reviewer said, is very interesting, the boron-doped Si-C offering 575 mAh/g versus the Si-C level of 323 mAh/g at 6.4 A/g. The reviewer also noted the lower charge transfer resistance of B-doped Si-C and the enhanced rate capability of Si-C composite.

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.

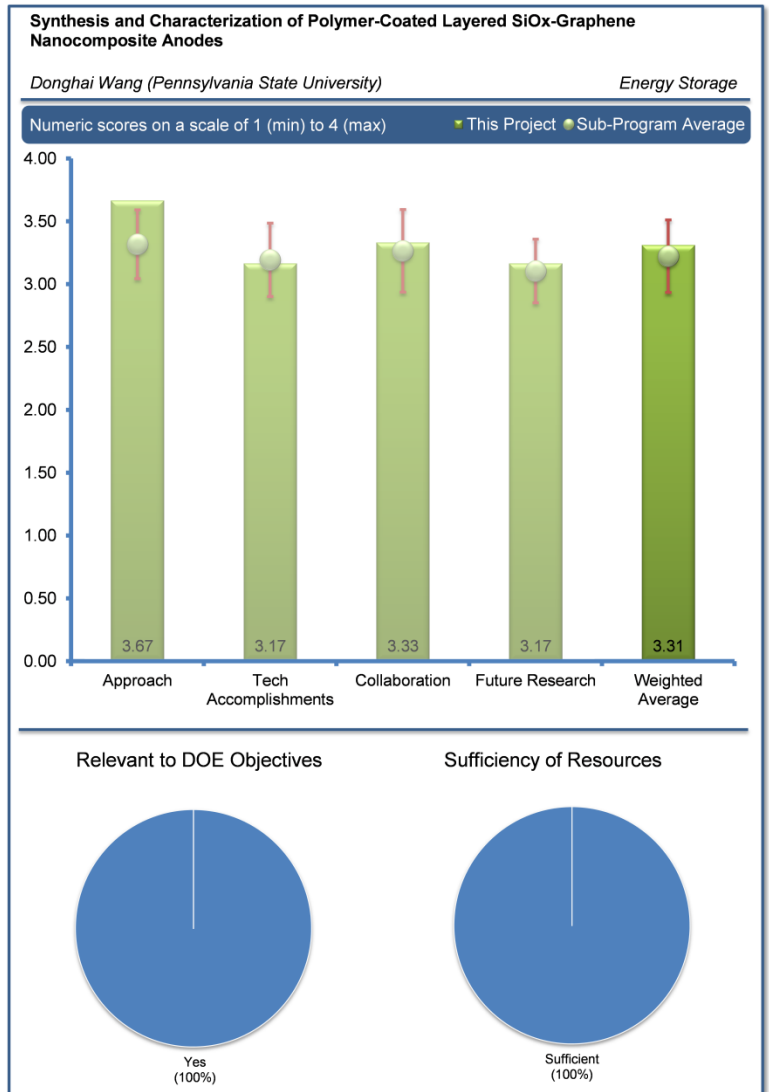
Reviewer 1:

Saying the investigators have done an excellent job on preparation of meaningful materials, the reviewer felt a more concentrated effort on merging the independent components into an electrode would have helped the program.

Reviewer 2:

This project has achieved some good progress, the reviewer stated, although capacity retention and charging efficiency appear still to be a big challenge, especially at low rates. It may be interesting, the reviewer conjectured, to see the impact of Si-C ratio in the composite on electrode performance.

Multifunctional binders with mechanical, ionic, and semiconducting functionality have been developed, the reviewer observed, and Si₂TiN seems to be a good candidate.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The PI has brought together some excellent researchers from different organizations to work together on this project, the reviewer said.

Reviewer 2:

Good collaboration was shown, the reviewer said, although in common with most presentations, the investigator had not clearly indicated what elements came from which collaborator.

Reviewer 3:

The collaboration with other researchers is good, said the reviewer.

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.**Reviewer 1:**

The reviewer felt the proposed work is reasonable and speculated that it may be interesting to see the impact of Si-C ratio on composite electrode performance in the future work.

Reviewer 2:

The reviewer observed that each task is well-aligned with previous work and felt it would be beneficial if the investigator begins evaluating multi-component systems (electrodes) utilizing the materials developed.

Reviewer 3:

Measuring surface interactions of functional polymers and Si composites and synthesizing new functional binders with acidic and semiconducting functionalities are good approaches, in the judgment of the reviewer, who also said postmortem analysis is needed.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The goals of this project are highly relevant to DOE objectives, in this reviewer's view.

Reviewer 2:

The research addresses the need for development of high specific-capacity anode materials for use in plug-in electric vehicles (PEVs), the reviewer stated, thus the focus on development of high-performance materials is appropriate, and the approach kept in mind the needs driven by PEV applications.

Reviewer 3:

This reviewer stated that the project reduces the use of petroleum.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

There are sufficient resources for this project, said the reviewer.

Reviewer 2:

The reviewer identified no issues and called the program well managed.

Reviewer 3:

Sufficient resources are available, the reviewer felt.

Wiring up Silicon Nanoparticles for High Performance Lithium-ion Battery Anodes: Yi Cui (Stanford University) - es148

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

This project is highly relevant to DOE objectives, in the judgment of the reviewer.

Reviewer 2:

The reviewer deemed the approach to be good.

Reviewer 3:

The project was well structured to address the major barriers, the reviewer stated, and the investigator recognized the need for high energy, cyclability, rate capability, and cost. A more structured approach to the cost analysis goals would have been beneficial, however, the reviewer said.

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.

Reviewer 1:

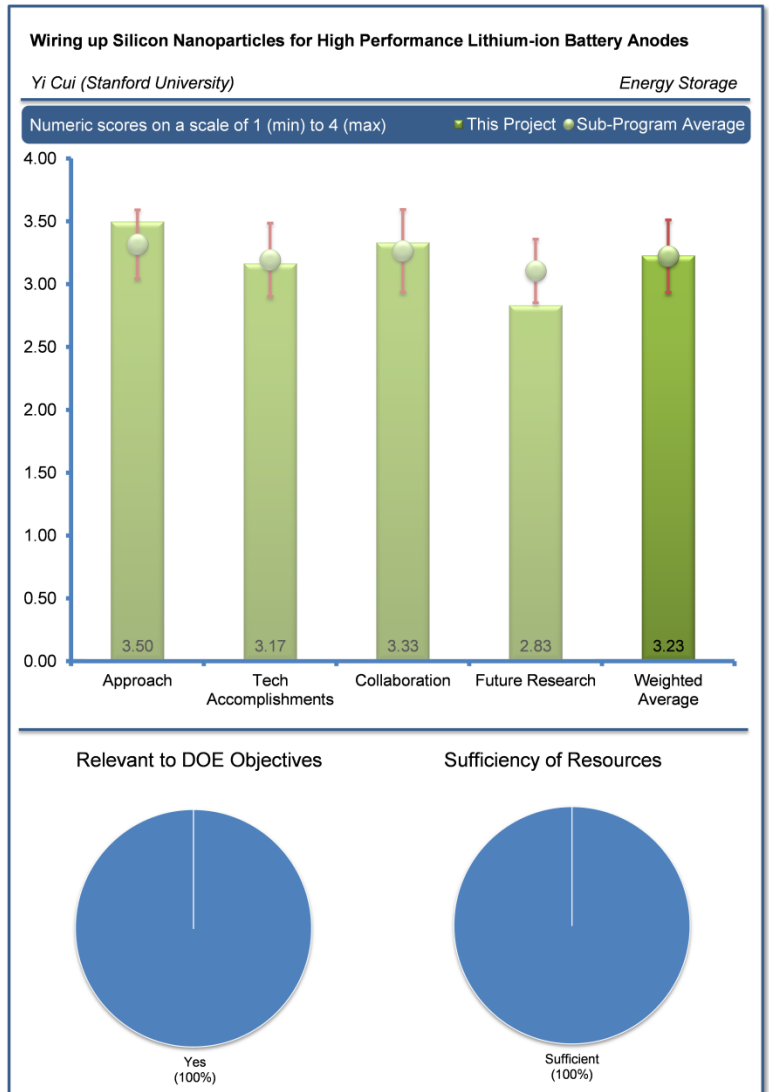
Terming the approach innovative and well-focused, the reviewer noted that the investigator applied different geometric approaches to address energy and cyclability. The research, the reviewer said, certainly suggests the next stage should be in effective electrode design, including binder selection and incorporation.

Reviewer 2:

This project has achieved numerous accomplishments, the reviewer said, but the low charging efficiency remains a challenge for the battery cycle life.

Reviewer 3:

The reviewer asked what the actual silicon loading is, noting that it has to be indicated, along with the current. Calling attention to Slide 8 of the presentation, the reviewer noted the importance of cost in making nanosilicon. While the source material is cheap, the question is processing cost, which should be addressed, the reviewer said. First cycle irreversible loss also has yet to be addressed, the reviewer noted.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

Excellent collaboration, the reviewer said.

Reviewer 2:

The PI has numerous collaborations with different institutions to work on this project, the reviewer noted.

Reviewer 3:

The reviewer said it was clear in the research presented that the teams were well coordinated.

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.**Reviewer 1:**

The reviewer believed the project team may need to address the charge efficiency challenge in the future work.

Reviewer 2:

The reviewer considered that an area on which the investigation needs to place significant focus is improvement of the coulombic efficiency over the first 50-100 cycles. This was an issue of great concern to the reviewer, since the electrode as shown would not be practical in a Li-ion cell otherwise.

Reviewer 3:

The reviewer inquired about the selection of micro-sized Si anodes with long cycle life.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This project is highly relevant to DOE goals, the reviewer said, and is targeting on attacking high anode design for battery applications.

Reviewer 2:

The team correctly identified the key needs for viable high-energy PEV cells, and addressed each in this project, the reviewer stated.

Reviewer 3:

This reviewer stated that the project reduces the use of petroleum.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

It appears, the reviewer said, that there are sufficient resources for this project.

Reviewer 2:

The reviewer commented that the resources were well balanced.

Reviewer 3:

The project has sufficient resources, in the reviewer's opinion.

Voltage Fade, an ABR Deep Dive Project: Status and Outcomes: Anthony Burrell (Argonne National Laboratory) - es161

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

This is an excellent approach to address the problem of voltage fade in layered-layered oxide material on a fundamental multidisciplinary level, in the view of this expert.

Reviewer 2:

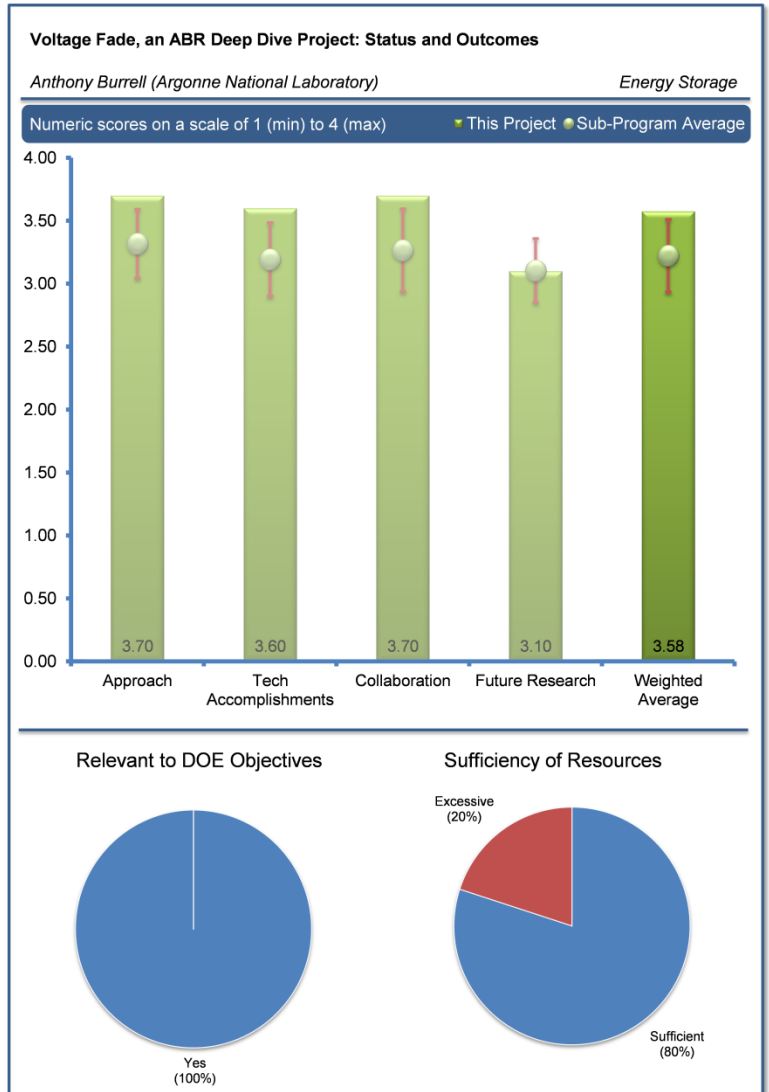
The team approach has been remarkable, in the opinion of this reviewer. The investigators clearly stated, the reviewer said, that voltage fade is intrinsic to these materials. Critical to a workable solution, in the reviewer's opinion, is to find a way by which some capacity can be traded for a lower capacity fade.

Reviewer 3:

In the opinion of the reviewer, the decision to form a large team to work on this key project has been validated by the tremendous success of the team in answering the key questions about the fade of the layered-layered cathode. The reviewer deemed this an extremely impressive effort, involving all disciplines and many organizations in many locations. The reviewer noted that there are many cases in which large teams burn through prodigious amounts of funding, but still really do not answer the key questions. Thus, the reviewer found the successful accomplishments of the project team very gratifying and felt that it shows that the DOE's confidence in this approach was well-placed. The program was obviously extremely well managed and a credit to the staff, the reviewer concluded.

Reviewer 4:

The reviewer characterized the presentation as an overview of the deep-dive program directed toward understanding, and potentially solving, the voltage fade problem of the LMR-NMC materials, using a team approach at ANL. To this end, the reviewer noted, an array of characterization techniques, electrochemical methods, systems and materials modeling were used, leading to a consensus among the ANL scientists about the causes and interactions between the observed hysteresis and voltage fade due to structural changes observed in several candidate materials. However, the reviewer expressed concern about the possibility of groupthink being an outgrowth of this type of approach, especially since there was very little involvement by other institutions (Oak Ridge National Laboratory being the primary exception). In view of the considerable work all over the world on LMR-NMCs, the reviewer said, there should have been opportunities to collaborate formally or informally outside of ANL, to serve as verification or repudiation of the theories that were developed.



Reviewer 5:

The project work would make significant short-term gains in battery materials, the reviewer stated, by stabilizing and improving known materials so they could see wider commercialization. The reviewer deemed it good that the protocol makes fade more likely and any solution should be robust.

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.**Reviewer 1:**

Overall, the reviewer said, a great deal was accomplished, showing that the team approach directed toward understanding a specific problem (voltage fade) worked well. After two years of effort, the details of the structural evolution of the LMR-NMC materials are better understood, although, the reviewer went on, it is clear this difficult problem cannot be solved, only mitigated. The question now, in the reviewer's opinion, is whether the steps taken to mitigate voltage fade (e.g., lowering the charging voltage limit during cycling and/or reducing the excess Mn content) also lowers the energy content to the degree that the LMR-NMC materials are no longer competitive against other cathodes like NCA. Although raw materials costs are lower for LMR-NMC than for NCA, the reviewer observed, if special electronics, coatings, and etc. are needed to get the former to work as needed; this may raise the overall cost.

Reviewer 2:

Calling the overall program's progress massive, the reviewer noted that it was all self-supporting, interlinked and reviewed. The reviewer deemed it excellent to pull in the major conclusions early and equally valuable to show what does not make a difference (e.g., coatings) and separating out confusing elements such as impedance.

Reviewer 3:

In the judgment of the reviewer, the project's excellent results reveal most of the underlying mechanisms and lead to a fundamental understanding. Limits and potential of the material are much better predictable and strategies/next steps can be reasonably defined, the reviewer said.

Reviewer 4:

The project team has basically answered the question about voltage fade, including showing what will not work to resolve the matter and pointing the way to what might work, the reviewer said. Accordingly, the reviewer went on, the team has greatly advanced the science behind the layered-layered material with a degree of thoroughness not usually attained in academic or industrial labs. Moreover, the reviewer added, the team has done this in a relatively short period of time. Personal experience, the reviewer said, has indicated that while having more money and people is helpful, it does not always guarantee a fast answer, especially in fundamental studies such as these. The reviewer noted some suggestions would be offered in the Proposed Future Research section, but said that, in fact it is hard to improve upon this team's work.

Reviewer 5:

Noting that the investigators' array of techniques to study the problem from different angles, the reviewer said integration of those results has produced a better understanding of the problems. It seems clear, the reviewer said, that voltage fade is unaffected by coatings and additives, and is a property of the LMR-NMC materials. The reviewer expressed hope that, based on those findings, the project team will be able to find a workable solution. Synthetic efforts should not be discounted, the reviewer concluded.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer cited this as probably the best example of true collaboration in personal recollection and called the project's management excellent, noting that these are not easy cats to herd into a real team.

Reviewer 2:

The reviewer noted outstanding coordination throughout the different teams.

Reviewer 3:

The reviewer cited impressive cooperation within the Voltage Fade Project which is delivering excellent results due to the input and cross-linking of the results of individual work.

Reviewer 4:

This has been an extremely impressive effort, the reviewer said, involving all disciplines and many organizations and locations. The reviewer termed the teamwork shown among the modelers, chemists, electrochemists, etc., as simply outstanding for the most part and called credit to both the management and the individuals involved. The project, the reviewer said, should serve as a role model for the DOE and other organizations on how to tackle thorny, difficult technical problems that are poorly understood. The reviewer's sole only complaint was about a perceived disconnect between the modeling work at Berkeley by Persson and the modeling and mechanistic studies elsewhere in the program. The two groups appear to have conflicting theories, the reviewer said, with the ANL group seeming to discount or ignore the modeling efforts at Berkeley. Finding no intrinsic problem with this, the reviewer nonetheless saw no attempt by either group to actually resolve any differences. If there is a disagreement, the reviewer urged it be resolved as a team, using science, logic and data.

Reviewer 5:

The deep-dive project clearly was a team effort among ANL scientists, to the point, the reviewer said, that it is difficult to fairly assess the contributions of individuals to the overall program. In a side note to program managers, the reviewer said that if a program is designed as a team effort, the entire team should be reviewed as a whole, rather than having separate reviews for each participant. Noting that the only outside collaboration was with ORNL on neutron diffraction experiments, the reviewer expressed a desire to have seen more formal or informal collaborations with researchers outside of ANL, since work on the LMR-NMCs is carried out at many places throughout the world. Collaborations with outsiders, the reviewer said, can serve as a needed check against groupthink in interpreting results.

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.

Reviewer 1:

The deep-dive project is ending this year, the reviewer noted, and future work is focused on wrapping up the project. A number of items listed in the Future Plans slide made it sound to the reviewer like work may continue in a different context (e.g., in a different program). If this is the case, the reviewer felt someone needs to take a hard look at the costs and benefits of studying these materials further versus investing some effort in other approaches or alternative materials that are competitive in terms of specific energy (e.g., improving cycle life of NMCs cycled to higher voltages).

Reviewer 2:

The authors and teams have honestly disclosed the issues related to voltage fade, the reviewer said, but unfortunately, it is becoming clear what not to do (coating, use of certain additives, etc.) to resolve this issue. It will now become more urgent to focus on workable solutions, the reviewer stated and synthetic efforts should also be pursued.

Reviewer 3:

The reviewer expressed a desire to see a similarly large attack devoted to seeking ways to stabilize the phases (not all paths were ruled out, the reviewer noted) or to encourage reversibility rather than fade.

Reviewer 4:

Excellent results should be objectively reviewed in order to determine the real potential of the material to meet DOE targets on battery energy density for xEV, the reviewer said, and eventually to define next development projects to realize the potentials. The reviewer urged a careful look at other targets like power density and in particular safety. The question of the voltage window usable in xEV application should be addressed, the reviewer said.

Reviewer 5:

Acknowledging DOE's goals of thousands of cycles for a PHEV battery, the reviewer expressed the opinion that some of the approaches to other aspects of fade could realize cycle life that was at least in the 100-300 range. This, the reviewer said, would be good enough for many consumer applications, especially as each cycle would be longer than that for a typical Li-ion cell. Establishing what the best cycle life could be using these approaches may be enough to start its being commercialization, the reviewer conjectured. Apart from the monetary aspects, the attention this would get from cell makers would greatly increase the number of researchers working to optimize the material, the reviewer continued, and leveraging the large staffs of the commercial enterprises might be the best way to address the problems for longer cycling that DOE needs. The reviewer called for a clearer effort to delineate the best cycle life currently achievable, even without fixing voltage fade. Plans to study the activation cycle are good, the reviewer said, but a critical gap seemed to be the need to quickly test and evaluate Tarascon's work on using ruthenium (Ru) and tin (Sn) doping to stabilize the cathode material. Finally, the reviewer again urged resolution of the perceived modeling disconnect between ANL and Berkeley.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The project is very relevant to the DOE objective of petroleum displacement, since LMR-NMC materials are candidate cathode materials for high-energy batteries needed for vehicle electrification, the reviewer stated.

Reviewer 2:

Yes it is, the reviewer affirmed succinctly.

Reviewer 3:

Yes, the reviewer said, the project helps advance a high-energy material to commerce. Moreover, it was devised at DOE, the reviewer added.

Reviewer 4:

The project helps to make available high-capacity cathode material in order to increase battery energy density and meet DOE targets on xEV vehicles, said this reviewer.

Reviewer 5:

This group, the reviewer said, has marshalled a huge array of resources to address the key problem with the layered-layered materials that has remained unanswered for almost 10 years and has provided a detailed and credible insight into this key material.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

Costs were not broken down by individual investigator efforts for this project, the reviewer noted, and \$4 million over two years is a more-than-healthy investment to make in the study of materials that are extremely problematic, due not just to voltage fade, but to other issues as well (low tap density, low rate capability, etc.). One could reasonably question, the reviewer opined, whether some of the money would have been better spent on development of other materials and materials discovery and spread out to other institutions, as well. The reviewer expressed a desire to have seen a more comprehensive comparison of the LMR-NMC materials to other possibilities (high-voltage spinel, high-capacity stoichiometric NMCs, materials containing two lithium ions per formula unit, etc.). Compare materials not just on gravimetric capacities, the reviewer urged, but also on densities, rate capabilities, electrode formulations necessary to overcome rate limitations (a high carbon content will compromise specific energy and energy density), stage of development, projected timeline to commercialization, etc. Only with this information, the reviewer asserted, is it possible fairly to assess whether this was money well spent. At the beginning of this program, the reviewer said, the argument could have been made that it was worth investing effort in LMR-NMCs because of the promise of high specific energy. Two years later, in the opinion of the reviewer, it is less clear that a similar, intensive effort is warranted in the future, since mitigating the voltage fade results in a lower specific energy and the materials still have other problems as well.

Reviewer 2:

The project had lots of cash, but because it was driving a very large amount of research, the reviewer noted (citing personal experience) that this is appropriate.

Reviewer 3:

This team approach, the reviewer noted, has of course demanded lots of time from many staff members and other research has naturally had to take something of a back seat. The reviewer approved of this choice, saying it was extremely effective. Going forward, the reviewer expressed the belief that this team can wind down and go back to doing more individual projects. In spite of this project's great success, the reviewer cautioned DOE not to let such a large team effort continue unless it is clearly still needed for this or some other critical problem. Sometimes, the reviewer noted, such large teams acquire a life of their own instead of breaking up when the job is done, or more correctly, when it is done sufficiently that the large team is no longer needed to work on it.

Overcoming Processing Cost Barriers of High-Performance Lithium-Ion Battery Electrodes: David Wood (Oak Ridge National Laboratory) - es164

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The team has accomplished the milestones for the first half of fiscal year (FY) 2014, the reviewer said, and is on track to complete the project on time (i.e., September 30, 2014). The reviewer described the main objective of the project as being to reduce the manufacturing cost by replacing NMP processing with water-based chemistry for all active materials, such as the LiFePO₄ cathode, the NMC 532 cathode, the ConocoPhillips A12 graphite anode, the NMC 532 and LMR-NMC cathodes and the Superior Graphite anode.

Reviewer 2:

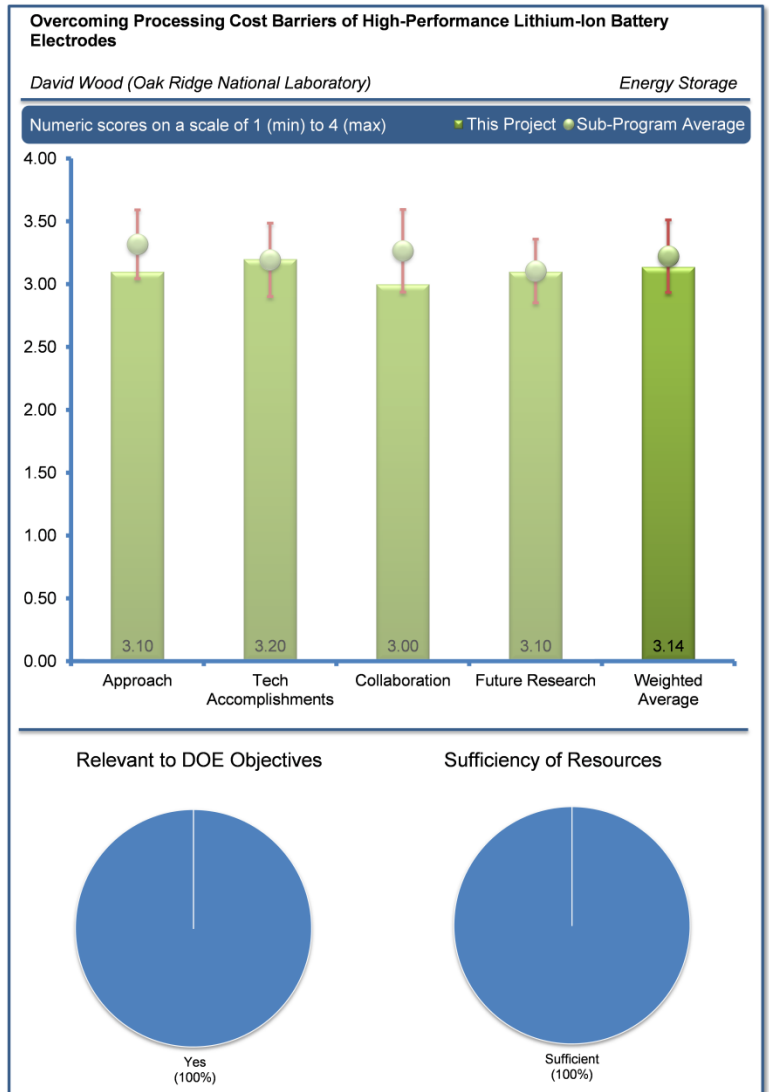
Avoiding use of toxic solvents is key to helping reduce costs and addressing a number of scale-up issues, the reviewer noted, adding that limitations on the use of water are being, or have already been addressed. This work is also helping to significantly reduce electrode processing costs and, indirectly, reduce current collector volume by producing thicker electrodes, the reviewer stated. The other key barrier addressed in this research is financial, the reviewer said, calling attention to Slide 8 which the reviewer felt nicely showed the key inputs to cost and their reductions achieved as a result of this research. Further identification of pathways that would drive down costs down to \$300/kWh would be desirable, the reviewer went on, but given the number of manufactured elements in a battery, this is not straightforward.

Reviewer 3:

The project is focused on transitioning electrode manufacturing to a water-based solvent system and the approach seems logical and measured, the reviewer said, as this is a process development activity much more than pure technology development. The evaluation of cell performance based on the process changes appears to be going well, the reviewer observed, calling Slide 8 detailing the cost improvement targets a welcome addition to the project, as this is in fact the actual goal of the work.

Reviewer 4:

Most of the gain is from thicker electrodes, which is not really new, the reviewer said. The project attacks processing problems, but these are not the big manufacturing barriers, in the reviewer's opinion. Expressing a desire to see proof of cost savings in actual application, not at hand scale, the reviewer said there is a need to move well past coin cells noting that full pouches were mentioned only once in the presentation. Also, the reviewer said, there should have been a full-scale electrode maker deeply involved from the start.



Reviewer 5:

Comparison of full cells using water- and NMP-based LiFePO₄ cathode and NMP-based CP A12 graphite anode shows comparable performance except for 1% less capacity retention in water-based cathode, the reviewer observed, asking if performance of the water-based anode formulation could be compared, also.

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.**Reviewer 1:**

The research has accomplished much in regard to water-based electrode preparation the reviewer said, calling this progress and the accompanying energy reductions noteworthy. The research is also poised to be successfully commercialized from the lab because of its large benefits and compatibility with existing equipment, the reviewer concluded.

Reviewer 2:

The team has established technology for aqueous processing of electrodes by blending colloidal and surface science with manufacturing science (coating, drying, etc.), the reviewer said. The team has demonstrated cycling performance in full coin cells and a 3-Ah pouch cell with water-based NMC 532 and CP A12 and has down-selected optimal waterborne polyvinylidene difluoride (PVDF) latex binder and determined optimal secondary drying protocol for aqueous processing the reviewer went on. The reviewer encouraged the project team to document and publish its findings in the open literature at the end of this project, especially those on water-based NMC 532/graphite electrodes. The team should also address whether aqueous corrosion is a problem for positive electrodes and methods of mitigating any such corrosion, the reviewer recommended.

Reviewer 3:

Milestone progress appears to be on track, observed the reviewer, who cautioned that, while the work at this level is very encouraging, its translation to large-scale, commercial processes, including different source materials etc., is still a large challenge.

Reviewer 4:

The project team has made good progress in all work streams, especially for the cost of the program, the reviewer judged. But the reviewer found it troubling that these electrodes have never been tested at high power, which is a major concern in thick electrodes and with new methods, since power really tests the cell's ability and durability.

Reviewer 5:

Noting that the capacity fade ranges are reported at 12-36% within 400 cycles, the reviewer said it would be desirable to compare the data for NMP-based cathode versus water-based cathodes.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

It is unclear from the publications and presentations by the project team what the value of this largest open-access battery R&D facility in the U.S. is to industry, in the opinion of this reviewer. The reviewer then asked if there were publications from the industrial partners.

Reviewer 2:

The reviewer observed that the project team has engaged a number of industry and laboratory partners, who appear to have helped in much of the material selection and loadings. The reviewer inquired about the current status of the licensees, but understood that, given the fluid nature of the situation, it may have been best not to comment in greater detail on this point.

Reviewer 3:

The list of collaborators appears broad and well-targeted, the reviewer said, although some direct feedback from partner organizations could be useful in validating the effectiveness of the program.

Reviewer 4:

The project has the right type of partners, although the reviewer would have preferred larger firms. The reviewer said it was unclear that there was much interaction with the battery partners, as only ANL is described as a close association.

Reviewer 5:

The reviewer felt there was excellent collaboration and coordination with other national laboratories and industries, but recommended adding academic research centers for some validation testing and fundamental studies.

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.

Reviewer 1:

The proposed future work is well thought out and logical, in the opinion of the reviewer.

Reviewer 2:

The closeout activities planned for the next couple of months represent a key process to transition this research from the lab to industry, stated this reviewer.

Reviewer 3:

Documentation and publication should be emphasized in the future work, the reviewer said, since the project is near its end.

Reviewer 4:

Calling the proposed future work the right work, the reviewer found it troubling that the scale-up supplier was not known and should have been involved from the start. There remains a lot to get done in four months, the reviewer noted.

Reviewer 5:

The project ends on September 30, 2014, the reviewer noted, finding it doubtful that the task on full cell fabrication and testing using water-based formulations for both anode and cathode materials can be accomplished in the time remaining.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

Reducing the cost for cathode material is essential, as it is for binders, and cathode materials are more expensive, the reviewer noted, calling this a highly relevant project for reducing the manufacturing costs of lithium-ion batteries.

Reviewer 2:

If project findings are true, a 20% reduction in battery costs would accelerate their deployment and ultimately the displacement of petroleum, said the reviewer.

Reviewer 3:

Cost improvement is a major requirement in the ongoing efforts to commercialize Li-ion batteries, the reviewer said and proliferation of these concepts into the commercial world will be a key goal.

Reviewer 4:

This work could help in manufacture but is really better aimed at U.S. Environmental Protection Agency (EPA) efforts to eliminate solvents, in the view of the reviewer.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer indicated that resources seem sufficient to distribute samples to partners, confirm the cost metrics, and ultimately make this work the new baseline by which to measure improvement.

Reviewer 2:

It is not clear, the reviewer felt, whether the team has already advanced enough to produce water-based anode formulations. If it has, the project could be finished in the prescribed time. Otherwise, it could require additional time and resources, the reviewer said.

Roll-to-Roll Electrode Processing NDE for Advanced Lithium Secondary Batteries: David Wood (Oak Ridge National Laboratory) - es165

Reviewer Sample Size

A total of six reviewers evaluated this project.

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.

Reviewer 1:

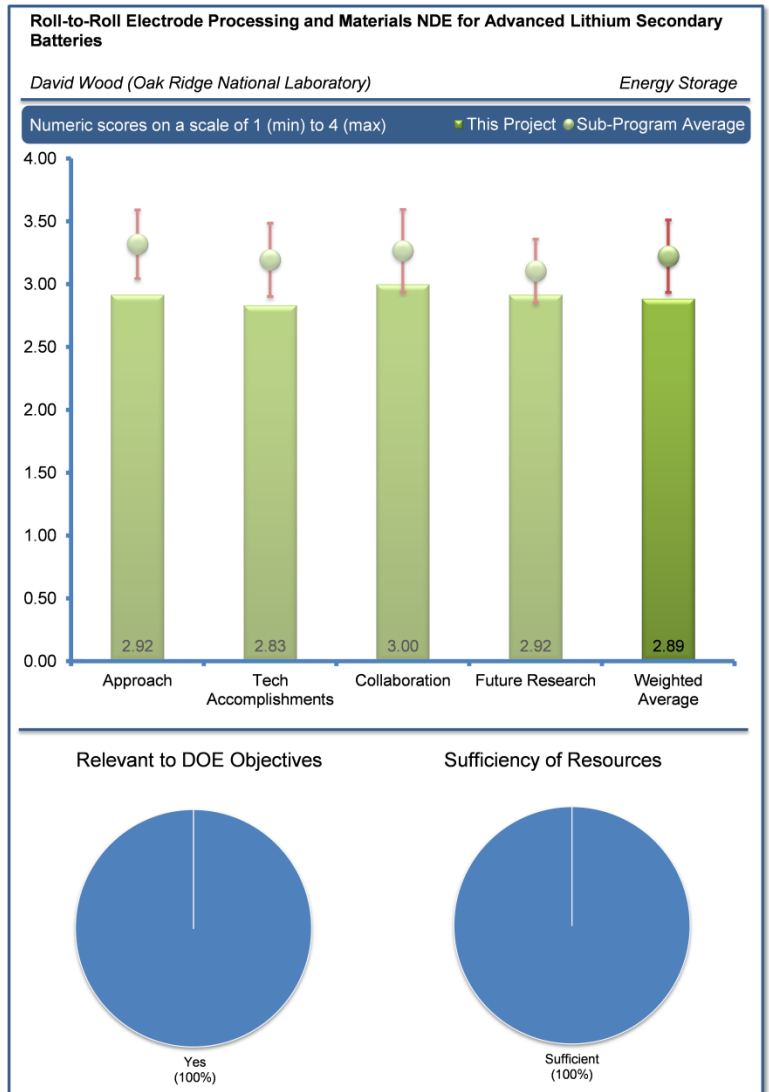
The project has employed a very methodical approach to improving cathode manufacturing scrap rates through advanced, on-line measurement systems, the reviewer stated, calling it vitally important that the validation for this as a critical, real-world, process issue be in place to demonstrate that coating improvement is a significant issue in commercial manufacturing. Given that assumption, the work here is well organized, highly detail-oriented and methodical, in the reviewer's opinion. The reviewer further expressed the belief that all reviewer comments from the previous year should remain a priority, since this is a highly complex subject and understanding which defects have which effects, as well as co-development of techniques to identify defects, is an extremely ambitious goal. These comments are simply a note on the scope of the project and should not reflect negatively on the capability of the group, which appears quite competent, the reviewer concluded.

Reviewer 2:

The team has evaluated several non-destructive evaluation (NDE) techniques for roll-to-roll lithium-ion battery (LIB) electrode processing, including cross-web laser thickness measurement, in-line X-ray fluorescence (XRF) and infra-red (IR) thermography, the reviewer observed. The results, the reviewer noted, are based largely on deliberately introduced metal contaminants and other intentionally introduced defects, such as pinholes, blisters, large agglomerates, and divots. During the final phase of the project (remainder of FY 2014), the team will scale cell testing of different coating defects to 1-Ah pouch cells for identifying which types of defects are critical to cycle life. It seemed to the reviewer that without knowing which kinds of defects are critical to cycle life, the approach of using deliberately or intentionally introduced defects is questionable, since these artificial defects may be unrealistic. The results obtained so far in this project may therefore not be meaningful, the reviewer felt. The project, in the reviewer's opinion should have started with identifying actual defects in commercial cells that are critical to cycle life before gathering data on deliberately or intentionally introduced defects.

Reviewer 3:

The reduction of scrap rates and increased utilization of active material directly reduces final manufactured costs, the reviewer pointed out, so addressing these issues sensibly reduces manufacturing costs. This topic is very important, the reviewer said, and expressed disappointment in the presentation of the research and the opinion that a better-scoped project would more clearly enunciate this value proposition. It does not appear, the reviewer went on, that any milestones or metrics speak to the progress toward meeting the 75%



recycle rate mentioned as the main objective. Also, the reviewer said, while all the research activities appear to address the issue broadly, they are again divorced from this top-level objective. The reviewer found this perceived disconnect between the approach and method, although not large, to be disconcerting. The project, in the reviewer's opinion, should have been scoped to have research efforts roll up quickly to the material and financial cost savings, and the awarded score reflects this oversight in the experimental design.

Reviewer 4:

The reviewer said the project had defined a limited set of defects to evaluate, established battery performance losses due to these defects and evaluated new concepts for detecting them in-process.

Reviewer 5:

Reducing scrap and thus lowering cost is a good aim, the reviewer said, and improved quality control (QC) and thus get more uniform cells is, also. The reviewer would have preferred a wider selection of collaborators, including more domestic battery makers and some end users on the team.

Reviewer 6:

The data shows excellent results, the reviewer opined, with full cells made using TODA H5050 cathode and Graphite A12 anode at a high voltage range of 4.7-2.5V having capacity of over 200 mAh/g up to 25 cycles, the reviewer observed. Cathodes, such as $\text{Li}^{1+x}\text{NiCoMnO}_2$, show high capacity at 4.7 V but capacity fade is also severe. The reviewer was unclear on how capacity fade was improved at higher voltage.

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.**Reviewer 1:**

The technical accomplishments are quite good, in the opinion of this reviewer.

Reviewer 2:

The results are based largely on deliberately introduced metal contaminants and other intentionally introduced defects, such as pinholes, blisters, large agglomerates, and divots, the reviewer noted. Without knowing which defect shapes, sizes, and compositions are critical to cycle life, the results obtained using deliberately or intentionally introduced defects may not be meaningful to the goal of developing non-destructive testing (NDT) techniques for quantifying the effects of different defect types on rate performance and cell lifetime of real-world lithium-ion batteries, the reviewer said.

Reviewer 3:

The reviewer questioned how the project can be only 75% complete if all FY 2014 milestones are on track, and whether this is a result of the no-go decision made last year. NDE of manufacturing processes should be quickly transitioned to industry partners, in the opinion of the reviewer, who said it is unclear that this has been done. This milestone was said to be completed in FY 2013, the reviewer observed, but no further comment was made on the subject. Getting to a pass/fail metric with some statistical significance would be huge in assessing and mitigating the risks of battery production, the reviewer said, and asked if there will be enough data to support this, referring to Slide 26. The correlation between defects and cycling data is starting to emerge, the reviewer noted.

Reviewer 4:

The project has elucidated how different types of electrode defects relate to battery performance losses, the reviewer said, and has begun to determine which detection methods may be effective for controlling processes and reducing scrap.

Reviewer 5:

Understanding the role of defects is being advanced with this program, according to this reviewer, who reiterated that the larger goal of quantifying and detecting defects is very ambitious.

Reviewer 6:

Progress seems okay, the reviewer felt, but when half the progress for the year is receiving and installing equipment and establishing methods, it has not been a banner year. The reviewer approved the no go decision, calling it honest. The project team showed that defects cause fade, the reviewer said, but did not find that surprising. The team was also able to make some optical method progress in partnership with NREL, the reviewer observed, expressing the hope that it was just hard to get the machines in and up to speed. The reviewer noted no measure of progress toward the goal of reduced cost.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

There were excellent collaborations with other labs and industrial partners, in this reviewer's judgment.

Reviewer 2:

The project has effectively blended collaborations with electrode material suppliers with equipment producers to accomplish its goals, in the opinion of the reviewer.

Reviewer 3:

Calling it very late in the project to be identifying an industrial partner to scale selected QC methods, the reviewer said industrial partner(s) should have been brought in earlier to comment on their capabilities and offer insights about deployment feasibility during the experimental design phase. Project collaborative activities could potentially be considered much higher if impact upon the partners' manufacturing lines (listed on Slide 17) was discussed, the reviewer commented.

Partners, and especially battery partners, in the reviewer's judgment, do not have obvious contributions other than discussion (which is not really collaboration). Work with NREL is more like partnership, the reviewer added, and only collaborations with national laboratories were described by the speaker as strong.

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.**Reviewer 1:**

This group consistently puts excellent thought into their technical direction, the reviewer said.

Reviewer 2:

The proposed future work is appropriate, the reviewer said, expressing the hope that it will be done on time, too.

Reviewer 3:

It is important to connect in-line monitoring data with battery performance data made using electrodes from the coater, the reviewer said and important to understand what the feedback loop control parameters are. It is also important to understand the extent of variations used as quality control for battery electrode fabrication using the produced coatings, something that needs to be elaborated, in the reviewer's opinion. The reviewer felt it was not clear why in-situ XRD and transmission electron microscopy (TEM) studies are important in this particular project.

Reviewer 4:

Identification of the sizes, shapes and types of defects critical to cycle life should have been done at the start of the project and should be a main effort before the end of the project, the reviewer said.

Reviewer 5:

Without an industrial partner, the reviewer was unsure how the commercialization is expected to proceed, noting that Slide 18 says one is still being identified. The reviewer was given to think the time frame for commercialization may be overstated and was also unsure

that enough data was available to support a pass/fail metric. The project team appeared to this reviewer to still be doing significant research which, while important, does not necessarily belong in the project closeout.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

Scrap reduction and improved manufacturing processes will clearly drive down battery costs, the reviewer said, calling it a good piece of low hanging fruit to be targeting.

Reviewer 2:

Market acceptance of battery-powered vehicles will require outstanding quality control in low-cost electrode manufacturing, the reviewer stated.

Reviewer 3:

Defect analysis can ultimately improve quality and cost of Li Ion batteries, the reviewer said.

Reviewer 4:

The project, which is aimed at a good goal – reducing manufacturing cost and improving quality – is the only scrap reduction program the reviewer is aware of in DOE's battery work.

Reviewer 5:

This project has high relevance in understanding whether we can improve our battery manufacturing process through in-line monitoring, the reviewer said.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The potential financial/manufacturing impact of this work is large, the reviewer said, and accordingly it is critical to the continued deployment of batteries into the vehicle marketplace.

Reviewer 2:

The principal investigators have access to adequate amount of facilities and resources to complete the project, in the judgment of this reviewer.

Reviewer 3:

The reviewer observed that no mention was made of program activities that would not be accomplished because of lack of resources.

Reviewer 4:

Because the program is basically over, the reviewer felt this question is not important right now.

Post-Test Analysis of Lithium-Ion Battery Materials at Argonne National Laboratory: Ira Bloom (Argonne National Laboratory) - es166

Reviewer Sample Size

A total of six reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that ANL has established outstanding capabilities for post-test analysis of lithium ion battery materials. The facility is available to help DOE's ABR, Batteries for Advanced Transportation Technologies (BATT) and USABC Programs and to help industrial battery developers better understand life-limiting mechanisms.

Reviewer 2:

The reviewer thought that the post mortem analysis of Li-Ion batteries after a use profile seems like a good contribution to the overall knowledge base of Li Ion chemistry. The approach appears rigorous and focused and is likely to add to our overall knowledge base. The reviewer felt that it is critical to both develop the techniques as well as the knowledge the project provide and this appears to be a well thought-out goal of the program.

Reviewer 3:

The reviewer pointed out that this is diagnostic work, but it was pitched as helping to inform rational research and design. As it progresses along it does not appear to have successfully completed (or begun) this second element to any significant degree.

The reviewer's rating reflected that much of these tests had already been performed in other laboratories. The key step forward would be in identifying what tests are truly diagnostic and worth of limited resources (time and money).

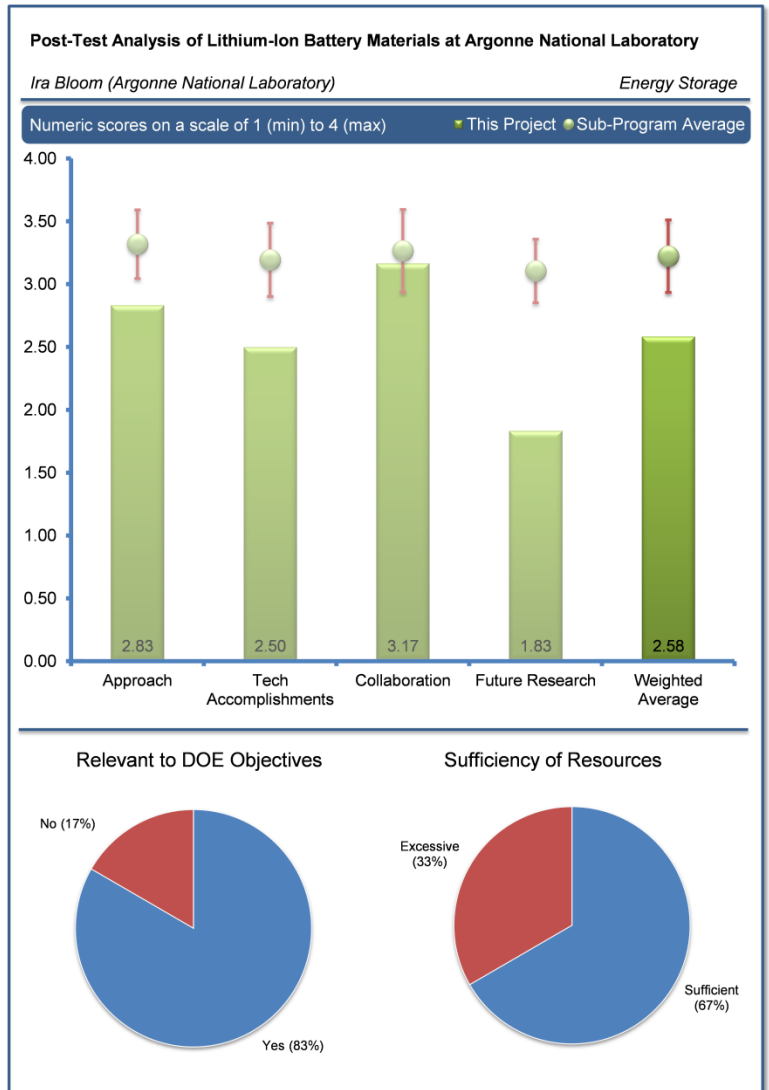
The reviewer recommends a clear focus on identifying key diagnostic tests and expediting this process to accelerate the feedback loop of rational design.

Reviewer 4:

The reviewer reported that the project has good infrastructure for Li-S, Li-Air, and Li-ion battery assembly facilities with well-equipped instruments.

Reviewer 5:

The reviewer regarded the concept to the approach to be fairly good in terms of trying to do tear downs and analysis to understand failure mechanisms in cycled cells, but the reviewer had major problems with the way this was being carried out. The reviewer first emphasized that this type of work was absolutely critical to the program. Also, it was actually very hard to do properly, especially when working with such air-sensitive materials. Having said that, the reviewer felt this presentation was simply awful from start to finish.



The reviewer listed eight specific problems, details of which follow. The first issue commented on by this reviewer was the inability to study cells at high state of charge – apparently for safety reasons. The reviewer would have thought the laboratory could have found a way to do this safely, especially for small cells. The reviewer added that maybe discharging them first could be the norm, but the reviewer would have thought that one would have to at least by exception look at charged cells to really understand what was going on.

The second issue commented on by this reviewer was the finding of lithium metal – if that is what it was – on a cell discharged to 2.0V was clearly very strange. The PI did not seem to find this odd, which in itself was something the reviewer found odd.

The third issue commented on by this reviewer was the inability to distinguish metallic lithium from lithium salts. This was a critical failure since metallic lithium was a clear sign of a cell malfunction. Offhand, the reviewer would have thought this could be gleaned just by placing a small sample in water and checking the solution for Li/F/P ratio, maybe also titrate for LiOH.

The fourth issue commented on by this reviewer was the lack of washing and even more so, the lack of a washing protocol. The PI seemed to think the cell submitters should work this out but, but this was clearly his job. Looking at a surface coated with salt in such excruciating and time-consuming detail seemed pretty pointless.

The fifth issue noted by this reviewer was determining the volume of gas (fluid immersion, inject a known amount of a reference gas, etc. The sixth issue commented on by this reviewer was whether the project team could not say anything about the FTIR peaks in terms of chemical bonds. The seventh issue commented on by this reviewer was where the origin of the fluoroethane. The eighth issue commented on by this reviewer was a lack of electrolyte analysis – just a gas analysis.

The reviewer went on to say that, this work, if done correctly, should cycle back and dictate future cell trials. For example, to determine where the fluoroethane comes from, a cell could be made with a non-fluorinated binder or a non-fluorinated salt to see if that stops the formation of fluoroethane. The reviewer expected that this kind of work could provide rich rewards if done thoroughly, but opined that this was not the way to do it.

The reviewer suggested that it should be done like competing product analyses. It does require a tremendous amount of work, even on one cell; the project did not appear to have even started to analyze the cathode or separator for defects in the cell(s) the team looked at. The reviewer wondered if maybe resources were an issue, but the results of this program were in the reviewer's view likely to be worthless unless major changes were made to the program.

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.

Reviewer 1:

The reviewer felt that the program was beginning to provide insight into common cause degradation mechanisms which should be valuable to the overall understanding of battery life.

Reviewer 2:

The reviewer stated that the ANL facility for post-test analysis of lithium ion battery materials had been used for a wide range of projects for collaboration with researchers working on DOE programs and industrial partners.

Reviewer 3:

The reviewer reported that there had been good progress with the original objectives. However, it would be good to recognize the most important objectives in terms of desired understanding in terms of post-test analysis.

Reviewer 4:

The reviewer thought that the approach was admirable, but so far little had been determined that informed failure mechanisms.

Reviewer 5:

The reviewer indicated that the example given drew major concern about the drying and decomposition of electrolyte salt on electrode not adequately considered in analysis.

Reviewer 6:

The reviewer categorized the results as mostly just data, no real interpretation, which was the single biggest complaint. The reviewer opined that this PI needed to step up, take ownership of this task, and really understand what was being found. Just passing on data back to the cell submitter is an abrogation of responsibility. The reviewer suggested that instead of relying on looking for patterns in lots of cells, to look at the few cells the project had and to start using chemical knowledge, partners, etc. to speculate on mechanisms and create plans to test the hypotheses. The reviewer stated that some of the results were highly dubious (metallic lithium in a discharged anode).

Question 3: Comments on Collaboration and Coordination with other institutions:**Reviewer 1:**

The reviewer cited excellent collaboration with cell manufacturers.

Reviewer 2:

The reviewer thought that there was excellent collaboration with industrial partners and others within national laboratories.

Reviewer 3:

The reviewer said that for this research the project has reached out to USABC, DOE and ANL to gather end of life cells to test. This was a positive step but a broader group would be desired. The reviewer further stated that the project has also attempted to make their resources and capabilities available to the broader battery community.

Reviewer 4:

The reviewer observed that collaboration appeared to be within the DOE community, although many other collaborators were listed, but not discussed. The reviewer considered it important for both the technique protocols and the information gained from these techniques is brought to the wider community.

Reviewer 5:

The reviewer reported that the project was at least getting cells from people, but the PI did not seem to have much knowledge of the cell history (over the wall mentality). While this may not actually be the case (hard to tell in the time allowed), it at least appeared to this reviewer that the PI needed to get more connected to the cell design and testing to fully understand what to look for in the cells and devise better ways to analyze samples and understand what it means – especially the latter.

The reviewer felt that there should be a clear plan for each cell worked out with the team so that the PI knows what to look for in each and why. To do a proper teardown and analysis is so time-consuming that one cannot possibly run every analysis on every cell. The reviewer did not see any evidence of such a plan, which was considered crucial to make effective use of this PI's efforts.

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.

Reviewer 1:

The reviewer felt sure there was a plan for forward work. However, it was not provided, therefore the unfortunate low score.

Reviewer 2:

The reviewer said the future research plan was not provided in the slides.

Reviewer 3:

The reviewer reported that no future work was described.

Reviewer 4:

The reviewer indicated that the work needed to get back to helping to inform battery researchers of the key technical barriers that needed to be addressed from both a material and manufacturing perspective.

Reviewer 5:

The reviewer mentioned earlier that it was important to refine the objectives in terms of type of desired understanding.

Reviewer 6:

The reviewer asserted that the presenter did not really say much except that testing on a lot more cells and looking for patterns would start. The reviewer totally disagreed with this approach and recommended that the team meet and figure out ways to do this better before the project wastes time analyzing another cell.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer commented that failure prevention is key to maintaining high energy battery systems that have long lifetimes. The project as pitched would do this. However, the reviewer felt its implementation has fallen short.

Reviewer 2:

The reviewer felt that without post-mortem analysis progress in improving battery performance is a blind operation doomed to move slowly.

Reviewer 3:

The reviewer believed that improvement in post mortem analysis is a worthy goal in improving our knowledge base.

Reviewer 4:

The reviewer indicated that this work should be highly relevant and critical to making progress. However, unless it undergoes a major shakeup, it will just generate large amounts of useless data.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer relayed that there did not appear to be any milestones, so could only judge this to be an inefficient use of limited resources.

Reviewer 2:

The reviewer declared that until this work program was completely revamped, no more money should be invested in any of this work. If and when properly directed and carried out, it will actually require a lot of resources, maybe even more than currently assigned. The reviewer concluded that the project was a long way from where it needed to be to justify any funding.

Process Development and Scale-up of Advanced Cathode Materials: Greg Krumdick (Argonne National Laboratory) - es167

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer felt that the approach was useful and met the objectives. However, there was little understanding of why scale-up resulted in synthesis of suboptimum electrolyte or active materials.

Reviewer 2:

The reviewer believed that the program had taken a well-considered approach to identifying targets and systematically characterizing synthetic products to meet a complex set of requirements.

Reviewer 3:

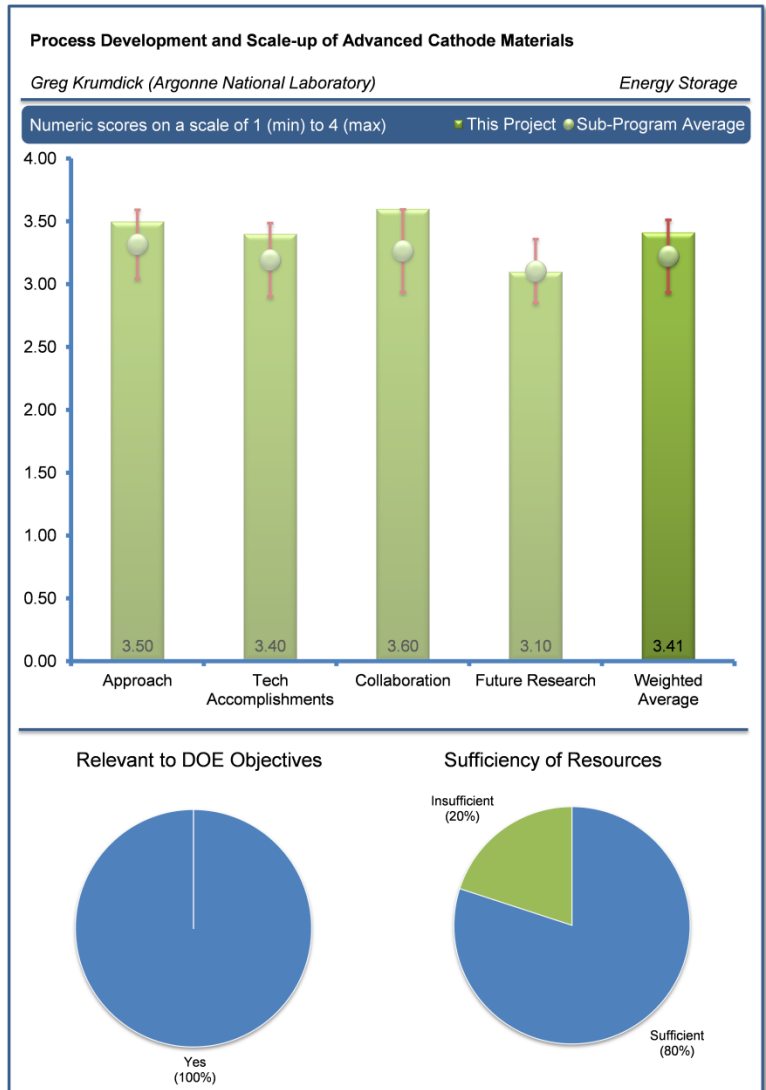
The reviewer found the technical approach to be well thought-out and competent, but respectfully suggested a concern about the place of this research within the community. There are a number of very large, multinational corporations who are in the business of supplying large scale amounts of cathode material and have incentive to provide lower cost, high quality materials as time goes on. The reviewer considered that finding a productive “niche” of DOE sponsored work in this area that complements the work in the community, or adds some specific value to the work of the community was perhaps a challenging task. If the goal is to provide advanced materials to the community in lieu of the sometimes difficult availability from commercial suppliers, this could be a worthy goal. If the goal is to “compete” at the process development level with the large multinational providers, the reviewer suggested that this might not be a very worthy goal.

Reviewer 4:

The reviewer asserted that the researchers have a clear understanding of the throughput limitations to scale up. Process optimization can be a never ending process, but they have put clear limits and are rationally targeting two materials per year to scale to multi-kilogram quantities. It appeared to the reviewer that the project team was currently slightly behind its target pace, but some of that might be expected to be the result of delays during start up.

The reviewer reported that the project team has clearly identified processes that could be scaled to larger quantities, and is targeting key steps to determine which factors are most important.

The reviewer commented that the only big thing is that the queue of materials to be optimized should already be clear. The next handful of materials should already be on the table, so that the input of industrial partners can be sought and if necessary brought on board.



Reviewer 5:

The reviewer suggested that target material number four should be identified. The reviewer recommended the design of experiments methods should be used for experiments involving a large number of parameters (e.g., Slides 8 and 10). The reviewer felt statistical data analysis should be used to see whether the 20% improvement in capacity at cycle 140 by 1% Al₂O₃ coating is statistically significant.

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.**Reviewer 1:**

The reviewer found that thoughtful execution of synthetic methods has led to scale-up of complex materials. The reviewer commented that inorganic synthesis in a continuous process is a particularly difficult and noteworthy accomplishment.

Reviewer 2:

The reviewer saw that the techniques being developed appeared to be showing promise as to their ability to produce advanced material concepts.

Reviewer 3:

The reviewer asserted that detailed understanding of fundamentals (i.e., effect of porosity, aspect ratio, and particle size distribution on tap density or effect of side-reaction on type of impurities in electrolyte) could benefit this project.

Reviewer 4:

The reviewer reported that the project has successfully scaled up two materials and are nearly completed with a third, all of which were of interest to industrial partners. The reviewer's demerit is for the belief that this research will not be able to finish an as yet unknown material by the end of FY 2014.

The reviewer noted in an aside that it would be ideal if there was a metric that tracked the impact of this process scale up work, potentially something that shows to what degree studies in the field have been accelerated due to the larger volumes of consistent starting material. The reviewer recognized that this was a non-trivial issue, but would likely make a strong case for this research.

Question 3: Comments on Collaboration and Coordination with other institutions:**Reviewer 1:**

The reviewer considered this to be a strong point of this research. The team and their industrial capabilities have even been sought by other companies who have brought in outside funding. The reviewer recognized this as a clear DOE programmatic goal.

Reviewer 2:

The reviewer claimed that collaborations within and between laboratories plus with the external customers were very good.

Reviewer 3:

The reviewer reported that partnerships were primarily focused on collaboration with other national laboratories. Expanding this field may increase program relevance.

Reviewer 4:

The reviewer noted that there is no collaboration with any commercial cathode material suppliers, which may or may not be the goal, but is noticeably absent.

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.

Reviewer 1:

The reviewer said that the planning, while logical in process, should have a more transparent process. The cathode material field, while evolving, generally has coalesced around several targets. The reviewer suggested that prioritizing these targets will help get more usable and broadly applicable testing data into the hands of researchers who will then be able to make appropriate decisions on the direction of research they take.

The reviewer concluded that it is key that the broader industry has a stake in what is being scaled up to maximize impact of the large quantities of material that will be available as an output to this research.

Reviewer 2:

The reviewer felt that the evaluation of emerging manufacturing technologies in particular seemed like a worthy goal of the group.

Reviewer 3:

The reviewer saw that goals appeared simultaneously ambitious and well considered.

Reviewer 4:

The reviewer could not see any clear path on how to decide the next project plus any critical-path analysis because the scope of objectives was very broad. Both could help with streamlining of activities toward objectives of the VTO.

Reviewer 5:

The reviewer asked if target material number four will be necessary as part of the future work.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer felt this project should help domestic industry to quickly and inexpensively have access to new R&D materials for their developmental activities for making better and more cost competitive energy storage systems.

Reviewer 2:

The reviewer said that scale-up of new materials would lead to more rapid identification of incentives and concerns for these materials by enabling extensive evaluation under more rigorous protocols.

Reviewer 3:

The reviewer concluded that careful management of the goals of the group would result in a program with a legitimate piece of relevance in the overall field.

Reviewer 4:

The reviewer pointed out that battery technology would only have an impact at scale, and thought that this work was a key step to making technologically advanced batteries at scale.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer judged that allocation of resources appeared to be adequate although details were not discussed. It would be interesting to the reviewer to know where the bottleneck is and how it can be resolved.

Reviewer 2:

The reviewer reported that this team looked to be progressing at just behind their proposed rate of two materials per year. The reviewer recommended that with optimization there be inherent scope limitations to maintain this rate until there is greater certainty in the selection of cathode materials.

Reviewer 3:

The reviewer concluded that the program had identified the quantity of materials that were likely to result at the current resource level. Increasing resources could potentially increase the number of materials that would become available from these scale-up efforts.

Process Development and Scale-up of Advanced Electrolyte Materials: Greg Krumdick (Argonne National Laboratory) - es168

Reviewer Sample Size

A total of six reviewers evaluated this project.

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.

Reviewer 1:

The reviewer noted that the scale-up and process development look good, but many of materials appear to be very expensive. The reviewer wondered about the cost target and any other concern such as toxicity and environmental issues.

Reviewer 2:

The reviewer found a disciplined, staged approach, which was unfortunately low on contact and partnership with industrial maker.

Reviewer 3:

The reviewer considered process scale-up to be a critical issue, and is being directly addressed in this research. However, the commenter indicated that more work needs to be done in prioritizing which chemicals/materials are scaled-up. The reviewer thought that, given the investment in each one, efforts need to be made in concert with battery

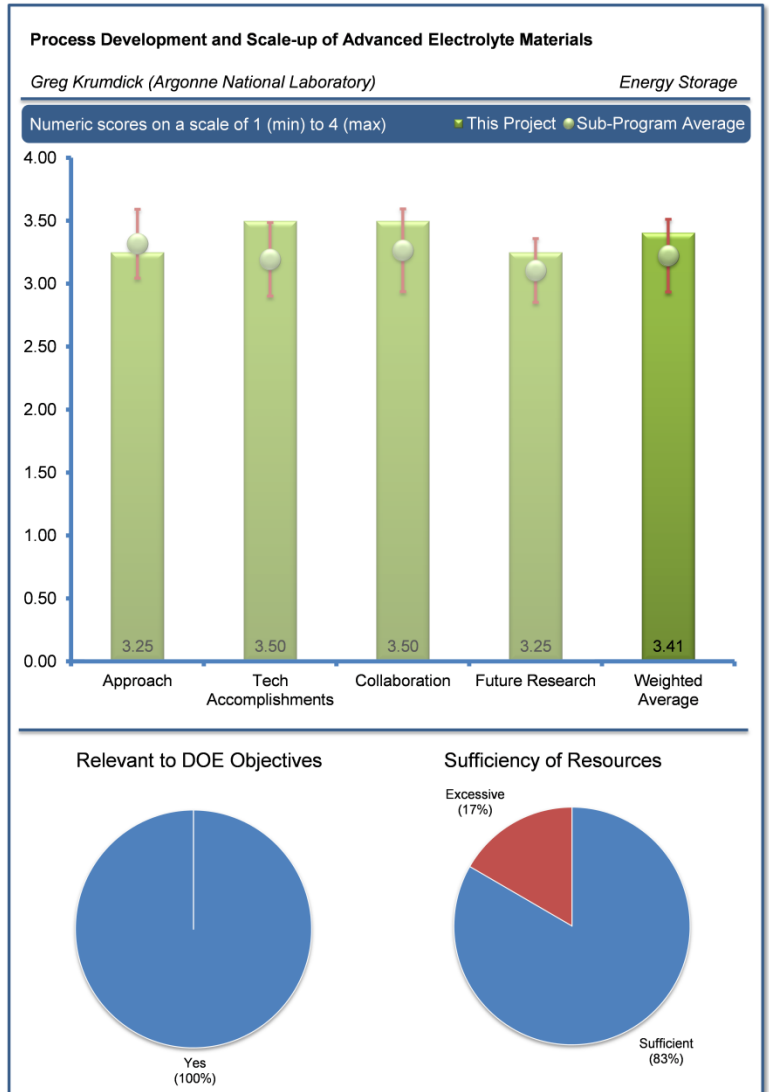
researchers to select materials with the greatest impact not available (in volume or quality) elsewhere. The project evaluator requested to have greater context to the material selection process as it is clear the researchers understand how to do process scale-up.

Reviewer 4:

The reviewer relayed that the group is responsible for developing synthesis schemes for promising electrolyte components such as salts, additives, shuttles etc. The commenter indicated that the capability appears to be sound, and that appropriate dissemination of the materials could clearly aid in the development of advanced electrolyte formulation concepts. The reviewer recognized that there has perhaps always been a question as to whether there is enough band-width in terms of the variety of synthesis approaches available to ensure that the most efficient approach is being used for each individual molecule. However, the reviewer stated that if the goal is fairly restricted to the ability to provide promising molecules, the results seem useful.

Reviewer 5:

The reviewer described that this project is about scaling-up production of electrolytes and make these materials available to various researchers.



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.**Reviewer 1:**

The reviewer acknowledged that this group has taken on an extremely challenging set of goals and has accumulated an equally impressive list of accomplishments. The commenter also noted that the evaluation of new materials was greatly enhanced by the availability of this scale-up work.

Reviewer 2:

The commenter noted that research continues to optimize processes for a number of high-priority electrolyte targets. The commenter agreed that this work is crucial in moving the field forward. The materials chosen are all high-priority targets and the reviewer generally agrees with their selection.

Reviewer 3:

The reviewer reported that it appears that a great deal of work has been carried out, but requested that the researchers to please not forget about the cost.

Reviewer 4:

The reviewer described that several interesting molecules were developed and provided for external testing. The commenter offered that, without an alternative source, this provides a useful service in the overall improvement of understanding to the community.

Reviewer 5:

The reviewer stated that the PIs made important progress with scaling-up a number of electrolyte materials and made them available to a number of researchers. Also, important finding were made in terms of the role of impurities.

Reviewer 6:

The reviewer said that the progress in nice, but for the funding one would also expect a lot of progress. The commenter pointed out that there were a diverse set of activities and progress on many fronts; however it was not clear to this person what the real meaning to industry and consumers is in terms of cost.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer recognized that the researchers extensively provided sample materials to various organizations.

Reviewer 2:

The reviewer praised that the growing list of collaborators is a good start. Even so, the commenter suggested that there is a continued need for collaboration to do two things: 1) help with standardizing the work in this field, and 2) prioritizing work to push materials into commercial production.

Reviewer 3:

The reviewer commended that this team has collaborated effectively with a diverse group of participants to make contributions in many areas of battery performance.

Reviewer 4:

The reviewer explained that the project collaboration scheme is complex, as there is collaboration on priorities, collaboration on testing and characterization, and ultimately in the decision making associated with both the technical and commercialization viability. The commenter offered a general comment that the visibility on the overall process of how materials are chosen, prioritized and dispersed would be a worthwhile endeavor. The reviewer acknowledged that this is not necessarily the responsibility of this particular group.

Reviewer 5:

The reviewer indicated that the researchers work with many people and there is give-and-take with partner contribution to the work at ANL and vice-versa.

Reviewer 6:

The reviewer simply stated that there was good interaction with a number of researchers.

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.

Reviewer 1:

The reviewer stated that prior to launch scale-ups, that the researchers should consider many other aspects beyond the functionality.

Reviewer 2:

The reviewer summarized that two key recommendations that appeared to be chief among the future research directions, as proposed by the team, are: 1) a need to better align this work with modeling efforts, and 2) clarify selection process. The reviewer highlighted that the consistent availability of high-quality materials will help to standardize research and data collection. The commenter stated that the ability for modeling experts to take this large quantity of data and create workable simulations could potentially accelerate development efforts. Thus, working with the modeling community to assess their data needs, would dramatically increase the impact of this research.

The reviewer asserted that the selection process is key to the impact of this work. The project evaluator also recognized that process development is a strength of this research team, but offered that it is clear their expertise lies outside of the battery community. The reviewer proposed that inviting feedback from the wider community and prioritizing targets will get stakeholder buy-in that means this research will move the needle.

Reviewer 3:

The reviewer explained that the need for this activity is underscored by the continued demand for more materials.

Reviewer 4:

The reviewer stated that as this project is a bit of a (highly technical) service, so the future research is basically more of the same as an ongoing activity, which the reviewer agreed was a good thing.

Reviewer 5:

The reviewer simply stated that the planned future research was appropriate.

Reviewer 6:

The reviewer stated that even though there has been good progress in terms of scaling-up production of several electrolyte materials, it is not clear whether there is any new knowledge in terms of scale-up techniques. The commenter noted that the role of impurities was discussed in terms of battery performance, but proposed that it would also be important to discuss the relationship between the scale-up and the amount of impurities in the materials produced.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer explained that there is a valley of death gap between laboratory and commercial scales, with much of this resting on choosing the right materials to carry forward. The commenter stated that larger quantities of choice electrolytes will enable the testing that commercial entities desire to make true investment decisions that will yield the next generation of batteries.

Reviewer 2:

The reviewer agreed that the scale-up of new materials will lead to more rapid identification of incentives and concerns for these materials by enabling extensive evaluation under more rigorous protocols.

Reviewer 3:

The reviewer confirmed that electrolytes are a clear priority in the improvement of cells. If no other source of development of exotic fine chemicals is available, this is a critical activity.

Reviewer 4:

The reviewer stated that the electrolyte is a big cost of, and barrier to, higher voltage and capacity maintenance both, so the work is definitely relevant.

Reviewer 5:

The reviewer commented that scale-up research is crucial for translating new materials discovery to marketplace.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer responded that the number of materials being synthesized seems reasonable for the current funding levels. The reviewer also suggested that there should be a clear future transition to industry funding (perhaps by a consortia of companies, or by research groups who purchase these chemicals.) The commenter emphasized that this statement is a future desire, and not a comment on the current funding levels.

Reviewer 2:

The reviewer claimed that the facility seems to have sufficient resources for the proposed research.

Reviewer 3:

The reviewer indicated that \$1.0 - 1.5 million a year for an electrolyte development project is a lot, as there are complete cell programs running for less. The commenter noted that while the researchers have a lot of work to do, it seems like this cost was not required.

In situ Solvothermal Synthesis of Novel High Capacity Cathodes: Feng Wang (Brookhaven National Laboratory) - es183

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that while the approaches for in-situ studies on synthesis and other diagnostic tests are novel, this person was not sure about those on high capacity cathodes.

Reviewer 2:

The reviewer noted that the approach was to develop new cathode compounds via controlled synthesis. The commenter explained that the approach also involved structural evolution of intermediates using in-situ reactors, coupled with time resolved XRD to identify reaction intermediates and reaction pathways to develop the capability to "dial-in" desired compounds and material properties. The reviewer stated that the experience will provide the insight to predict structure, etc., using the synchrotron X-ray facility and tracking of the lithium transport.

Reviewer 3:

The reviewer noted that in-situ XRD/XAS can provide critical information about synthesis reactions in real-time, which ultimately will be used, to develop useful phase diagrams.

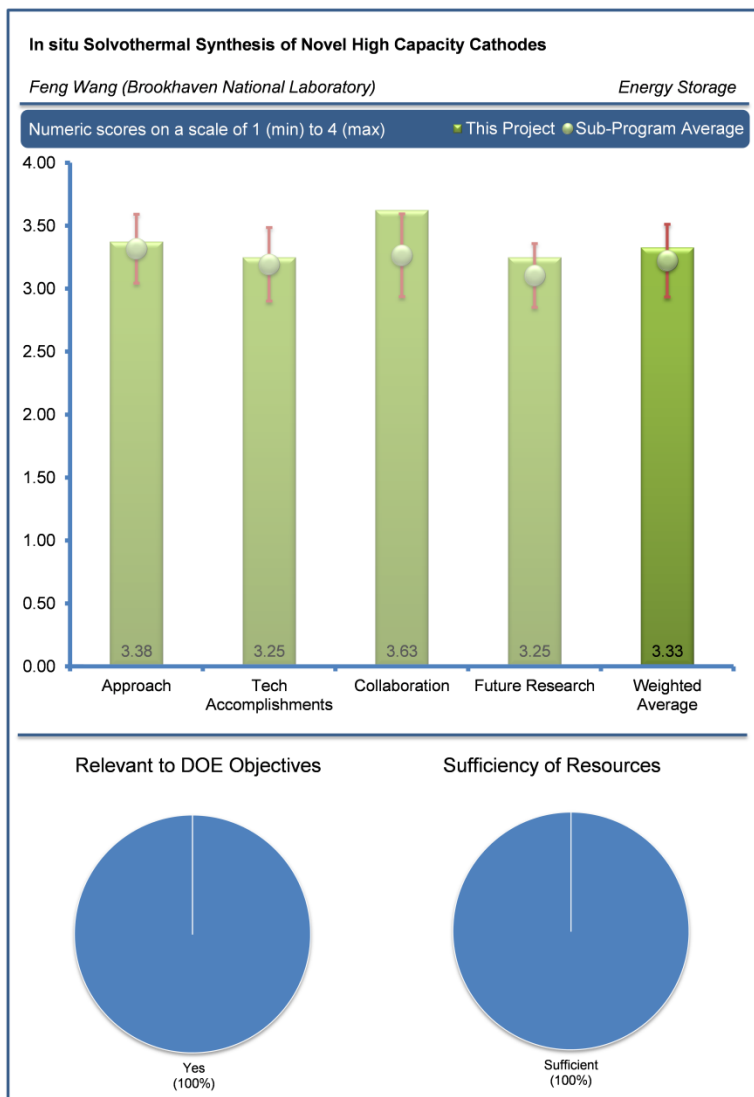
Reviewer 4:

This reviewer observed that the objective is to develop high-capacity cathodes, including Cu-V-O compounds, Li(Na)VPO₅Fx, Li-V-PO₄ and Li-Fe-Mn-PO₄. The approach, as reported by this person, is based on developing in-situ solvo-thermal synthesis to establish structure-property correlations and perform diagnostics for performance loss. The reviewer explained that the in-situ synthesis enables controlled synthesis of cathodes of desired phase and properties and is based on a combination of specialized in-situ reactors and time-resolved XRD probing for quantitative understanding of structure/phases during syntheses as well as during further lithiation-delithiation cycling. This reviewer further commented that the approach adopted here is useful in the development of new materials, but the choice of the cathode materials is not as beneficial. The reviewer added that the Cu-V-O system is not new, while the Li-Fe-Mn-PO₄ system is sufficiently mature and has low specific energy.

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.

Reviewer 1:

The reviewer reported that advanced X-ray techniques were used to synthesize new alpha-CuVO, LiFeMnPO₄F, and LiVPO₄(-X) cathode materials. An in-depth structural and electrochemical analysis of new high capacity cathode materials was also performed.



Reviewer 2:

The reviewer commented that in-situ XRD/XAS methods were developed and demonstrated; however, the analysis for identifying structures and crystallinities during the synthesis process have not been fully explored.

Reviewer 3:

The reviewer claimed that the diagnostic and the in-situ analysis data are extensive and quite useful; however, the reviewer criticized that the results from the new types of high capacity cathodes are not significant. The commenter asserted that cathodes with such low voltage and with so many plateaus are not attractive.

Reviewer 4:

This reviewer stated that good progress has been made towards developing the solvo-therml synthesis of ϵ - $\text{Cu}_x\text{V}_2\text{O}_5$ (ϵ -CVO) cathodes using in-situ XRD techniques and understanding their structural changes and limitations for extended cycling. Further, procedures were developed for the synthesis of α - CuVO compounds with new structure using both hydrothermal and solid state reactions, which were shown to give high capacity of 350 mAh/g with some cycling stability. The reviewer continued that these synthetic methods were also extended to two other cathode systems, LiFeMnPO_4 and $\text{Li}(\text{Na})\text{VPO}_5\text{F}$, and gathered useful structural information from in-situ XRD and EXAFS on these materials. Overall, opined this reviewer, these studies are interesting from an academic perspective, but do not add much value from the application perspective. The materials do not seem to meet the high specific energy/energy density requirements of the ABR.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer noted that the team comprises the best of the relevant laboratories.

Reviewer 2:

The reviewer reported there were extensive discussions and collaboration with the BATT program as well as external partners.

Reviewer 3:

The reviewer opined that this is a good, collaborative project involving interactions with several laboratories and universities.

Reviewer 4:

The reviewer simply noted that a long list of international collaborators were included.

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.

Reviewer 1:

The reviewer noted that the future work will continue the synthesis of new compounds and the characterization of high capacity cathodes with emphasis on polyanion-type materials.

Reviewer 2:

The reviewer agreed that the proposed future works are a logical step; particularly, on exploring the phase diagram research.

Reviewer 3:

The reviewer suggested that more focus on in-situ and other diagnostic studies, and much less emphasis on synthesis, should be given.

Reviewer 4:

The reviewer reported the following future plans: continue the investigation of $\text{Li}(\text{Na})\text{VPO}_5\text{F}_x$ cathodes to further explore the phase diagram in the space of temperature and Li concentration, emphasizing that this would be done via in-situ ion-exchange studies; develop new polyanion-type ternary and quaternary lithium vanadium phosphates cathodes (i.e., Li-V- PO_4 cathodes); investigate the new α -

CuVO cathodes further and test them in Seeo's polymer electrolyte; and develop advanced diagnostic techniques for studies of synthesis reactions during preparation of cathode materials and lithium reactions in electrodes. This person concluded that while these plans are consistent with the previous activities of this project and help ABR in developing new synthetic options for material development, the materials themselves are not that promising.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer pointed out that having a good understanding of the synthesis and failure mechanisms are critical for the development of state-of-the-art cathodes.

Reviewer 2:

The reviewer agreed that the fundamental approach for identifying and developing new compounds is essential for success of the DOE programs.

Reviewer 3:

This reviewer commented that low specific energies and high costs are the limitations of the current Li-ion batteries for EV applications. The reviewer indicated that several engineering improvements have contributed to a marginal increase in specific energy recently, but new high specific materials are desired to fill the gap. This person further explained that state of art cathode materials provide capacities of only approximately 160 mAh/g, which is about half of the capacities possible from the carbon anodes. The reviewer observed that the present project is aimed at developing new cathode materials with significantly higher specific energy.

Reviewer 4:

The reviewer said develop high capacity high voltage cathode for Li-ion batteries.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer stated that the resources are adequate.

Reviewer 2:

This reviewer stated that resources are adequate for the scope of the project.

Lithium Bearing Mixed Polyanion Glasses as Cathode Materials: Andrew Kercher (Oak Ridge National Laboratory) - es184

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer indicated that although this is a high-risk project, it has the potential of characterizing a new class of materials for their suitability as cathode materials. The commenter noted that approaches to tailor the voltage as well as the conductivity are certainly obvious and should remain the focus of the work. The reviewer also voiced that studies with inexpensive raw materials and low-cost processes should be always kept in mind.

Reviewer 2:

This person indicated that mixed polyanion glasses are expected to alleviate the problems faced with traditional crystalline polyanion cathodes (e.g., LiMnBO_3 , LiCoBO_3 , and $\text{Li}_2\text{CoSiO}_4$), such as poor conductivity and irreversible phase transitions. The reviewer noted that the objective here is to synthesize and mixed polyanion glasses in the phosphate family containing a variety of transition metal cations to have specific energies exceeding LiFePO_4 . The reviewer specifically identified vanadium substituted iron phosphate glasses [i.e., $\text{Fe}_4(\text{P}_2\text{O}_7)_3$ with 30-50% vanadate], which was shown to dramatically improve the specific capacity and rate performance. The approach is consistent with the objectives of this project as well as the goals of the ABR program. The reviewer commented that the approach is well integrated with the other materials-based efforts and appears feasible.

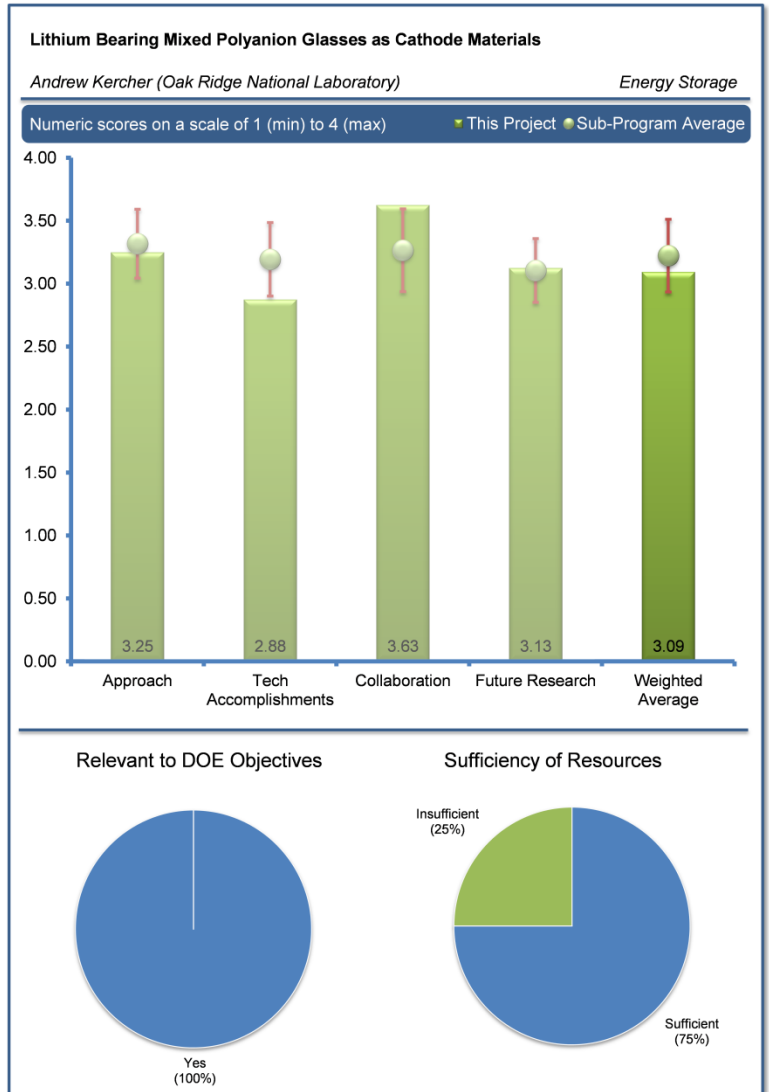
Reviewer 3:

The reviewer summarized that the approach is to synthesize and characterize electrochemical properties of polyanion cathode. The reviewer asked whether the carbon coating can be applied to polyanion cathode materials for improving the performance like LiFePO_4 .

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.

Reviewer 1:

The reviewer noted that reasonably good progress has been made in synthesizing and evaluating the vanadium substituted iron-phosphate cathodes in glass state. High capacities have been realized at lower voltage involving glass state reaction or reduction to Fe. However, this reviewer observed that the cycle life for the second reaction is rather poor. In addition to the iron phosphate glasses, several other multi-electron redox cathodes such as Mn and Co-bearing polyanion cathodes were synthesized and evaluated, but this reviewer reported



that the expected high capacities are yet to be realized in laboratory tests. Overall, the reviewer commented that the benefits from the mixed polyanion glass compounds are not significant compared to the crystalline analogs or other cathode options under the ABR program.

Reviewer 2:

The reviewer expressed that the first series of glasses that were synthesized were interesting, but the reviewer was quite curious to see how the particle size affects the charge/discharge capacities. Also, the commenter asked whether it possible to carbon-coat the materials to augment the electrical conductivity. The reviewer asked if the authors with synthesize the materials predicted by the simulations and try to analyze whether there is any agreement between the model and actual materials.

Reviewer 3:

The reviewer stated that only limited experimental results were demonstrated. It was not clear to this person what new significant understanding on polyanion cathodes has been gained from this study.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer acknowledged that there is an excellent synergy among all of the collaboration partners.

Reviewer 2:

The reviewer stated that the PI has developed collaborations with BNL on X-ray diffraction and Northwestern University on modeling.

Reviewer 3:

This reviewer noted that there are good on-going collaborations with Massachusetts Institute of Technology (MIT) and Northwestern University on the XANES characterization and modeling of these cathode materials, respectively.

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.**Reviewer 1:**

The reviewer recommended that the researchers please not focus too much on extensive cell making and testing. Rather, the reviewer suggested focusing on more new materials and identifying their characteristics and failure modes.

Reviewer 2:

The reviewer stated that if the PI believes that the ion diffusivity is the limiting factor, then experiments, such as EIS and NMR, should be designed to probe this issue.

Reviewer 3:

The reviewer reported that proposed future research involves continued development of a series of mixed polyanion glasses as a function of polyanionic substitution. The plans, continued this reviewer, are to synthesize, characterize, and perform electrical testing on at least four different glass cathode compositions with theoretical specific energies exceeding LiFePO₄. As an example, this reviewer noted LiMn ($\frac{1}{2}$ P₂O₇ + $\frac{1}{2}$ V₂O₇) with greater than 800 mWh/g theoretical capacity and LiCu($\frac{1}{2}$ PO₃ + $\frac{1}{2}$ VO₃)₃ with greater than 600 mWh/g theoretical capacity. The reviewer explained that equilibrium voltages for the glass-state conversion will be determined using galvanostatic intermittent titration technique. Though these studies look promising in principle, the reviewer indicated that practical specific energies will not be attractive because of the low capacities and voltages for the second reaction. The reviewer concluded that proposed studies are logical, but will fall short of addressing the technology barriers.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This reviewer opined that the limited range and higher cost of the Li-ion batteries are serious impediments for their use in electric vehicles. High energy density electrode materials will result in improved specific energy for Li-ion cells, increased range for the vehicle, as well as reduced overall cost for the battery. The reviewer further noted that state of art cathode materials provide capacities of only approximately 160 mAh/g, which is about half of the capacities possible from the carbon anodes. This person identified a need to develop new cathode materials of higher specific capacities, possibly with multi-electron redox processes, which is being addressed in this project.

Reviewer 2:

The reviewer simply stated the project was aimed at developing high capacity and high voltage cathode for Li-ion batteries.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer asserted that since it is a new class of materials with good opportunities, they would have funded it at a higher level.

Reviewer 2:

The reviewer indicated that resources are adequate for the scope of the project.

NMR as A Tool for Understanding Voltage Fade in LMR-NMC: Baris Key (Argonne National Laboratory) - es187

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer applauded that the approach was very good; NMR is one of the few tools we have to directly observe the local environment of Li-ions in materials, since Li is nearly transparent to X-rays. The commenter explained that disordering of the LMR-NMC materials could be directly observed using NMR, and Li-ions in different environments were quantified as a function of state-of-charge and cycle number. It was particularly interesting to the commenter to see direct evidence of Li in tetrahedral sites in the cycled electrodes.

Reviewer 2:

The reviewer emphasized that this mechanistic work has the most chance of identifying the problems source and fixing it. The commenter noted that the project is well-aligned with DOE's goals of getting vehicles with high driving range in the field.

Reviewer 3:

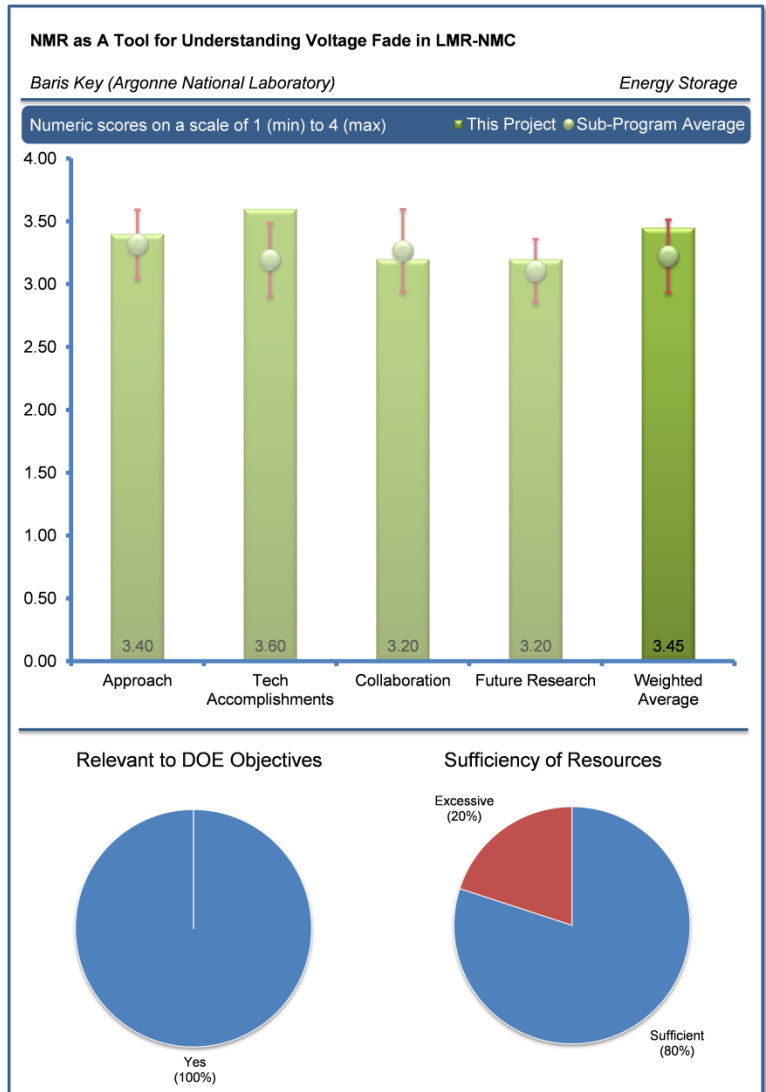
The reviewer commented that a very good analytical approach was used to reveal the mechanisms along the structural change of the layered-layered material under charge and discharge.

Reviewer 4:

The reviewer affirmed the good use of NMR to look at the local Li environment. The commenter highlighted that this provides information that cannot be attained in other ways, so complements other techniques. The commenter also noted that the technique can be used to study both domain types in the layered-layered cathode material. The reviewer explained that the technique helps to show what is really going on and samples a decent amount of the sample, so data are likely representative of the majority of the material.

Reviewer 5:

The reviewer suggested that at some point it should be very interesting to correlate the NMR data with Extended X-Ray Absorption Fine Structure (EXAFS) and additional theoretical calculations to see if it is possible to find or formulate general rules that can be used by the experimentalist as guidance for their research efforts.



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.**Reviewer 1:**

The reviewer affirmed that the project made good progress and accomplishments. The commenter explained that pristine and cycled materials were both examined as a function of state-of-charge and cycle number. The reviewer explained that the NMR and materials modeling work were complementary, with the experimental observation of tetrahedral Li being corroborated by DFT calculations.

Reviewer 2:

The reviewer praised that the authors have done a very good job with this sophisticated technique. The project evaluator suggested that it should be of interest to study also at least one standard material, such as NMC 111 or NMC 523, so the researchers can build and have a more wider “database” in relation to the Li behavior of these oxides.

Reviewer 3:

The reviewer highlighted that the return of Li to a disordered state is an important observation. The commenter offered that the role of transition metals migration is also important. The reviewer explained that these were all found with a lot of work completed and well-interpreted. The reviewer also recognized the researchers’ nice insight on the mechanism and the reason it slows down with time.

Reviewer 4:

The reviewer noted that the researchers showed transition metal migration as the cathode cycles. The commenter also reported that the researchers eliminated hydrogen insertion as a cause of voltage fade. The reviewer summarized that the researchers provided an excellent interpretation of the data via difficult analyses, squeezing all they can from the data.

Reviewer 5:

The reviewer pointed out the very good results that give valuable insight into the structural changes along cycling.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer recognized that the deep dive project really was a team effort. The NMR work was particularly well-coordinated with the electrochemical characterization (Abrahams), the materials modeling work (Adir), and with other efforts at ANL. The reviewer indicated that there was some coordination with ORNL on neutron diffraction experiments, but otherwise not much was done with other institutions. The commenter said that it would be have been nice to have seen a project like this opened up more to other national labs and universities to avoid the risk of “groupthink.”

Reviewer 2:

The interaction with a synthetic group should continue; it is very important.

Reviewer 3:

The reviewer stated that as with others good collaboration with a big team.

Reviewer 4:

The reviewer acknowledged the excellent cooperation within the Voltage Fade Project.

Reviewer 5:

The reviewer stated that the project has good linkage with ab-initio modelling at ANL and leverages other work like XRD data. The reviewer, however, cautioned that the project seems disconnected from ab-initio modeling work by Berkley (Persson, Project Number es091).

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.

Reviewer 1:

The reviewer indicated that the deep dive project is ending this year and that some future plans are focused on tying up loose ends, but others (e.g., providing local structural information to guide the synthesis work) sound like they are carrying over to other projects focused on the LMR-NMC materials.

Reviewer 2:

The reviewer praised that the future study using EPR is a great idea. This person also acknowledged that the study of the activation and first discharge of these high capacity powders is very important. The reviewer suggested that it should be interesting to study more established NMC cathode powders to contrast those results with the new high capacity powders.

Reviewer 3:

The reviewer explained that the future plans are to extend the investigation to different compositions of transition metals, and eventually dopants to further support the other experimental teams.

Reviewer 4:

The reviewer agreed that the researchers are targeting the right things. The commenter offered that it would be especially good to better understand the first cycle activation of this material, which seems to be very poorly understood.

Reviewer 5:

The reviewer simply stated that the future plans are in the right direction, but need definition.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed this work is very relevant to DOE objectives of petroleum displacement since LMR-NMC materials are candidate cathode materials for high-energy batteries needed for vehicle electrification.

Reviewer 2:

The reviewer explained that the project has enabled DOE premier work in the past and supports range/durability in applications to vehicle.

Reviewer 3:

The reviewer commented that the project helps to make available high capacity cathode materials in order to increase battery energy density and meet DOE targets on xEV vehicles.

Reviewer 4:

The reviewer commented that the project provides a new window into the structure of the cathodes as they charge and discharge.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer explained that the costs were not broken down by individual investigator efforts for this project. The commenter explained that \$4 million over two years is a more than “healthy” investment to make in the study of materials that are extremely problematic, not just because of the voltage fade issue but because of other issues as well (low tap density, low rate capability, etc.). The reviewer suggested that one could reasonably question if the money would have been better spent on development of other materials and materials discovery and be spread out to other institutions as well. The reviewer would have liked to have seen a more comprehensive comparison of the LMR-NMC materials to other possibilities (high voltage spinel, high capacity stoichiometric NMCs, materials containing two

lithium ions per formula unit, etc.). The reviewer also requested the researchers should compare materials not just based on gravimetric capacities, but also densities, rate capabilities, electrode formulations necessary to overcome rate limitations (a high carbon content will compromise energy density), stage of development, projected timeline to commercialization, etc.; only with this information is it possible to make a fair assessment on whether this was money well-spent or not.

Reviewer 2:

The reviewer could not say, and noted that this information was not provided.

Electrochemical Characterization of Voltage Fade in LMR-NMC cells: Daniel Abraham (Argonne National Laboratory) - es188

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer commented that the approach was very good. The commenter suggested that this talk should have come first in the schedule, as it was directed towards demonstrating and defining the problem of voltage fade in the LMR-NMC materials through a series of electrochemical experiments. The project evaluator described that periodic short current interrupts during cell charge and discharge were used to estimate the degree of voltage fade due to structural changes during cycling, and to distinguish this from voltage changes due to rising cell impedance. (The long time required to approach equilibrium, particularly at the end of discharge, means that it is only an approximation, however). The reviewer explained that LMR-NMC materials were compared to NCA and NMCs, which undergo much less true voltage fade during cycling to high voltage limits, clearly demonstrating what the problem is with the former set of materials.

Reviewer 2:

The reviewer reported that the authors have presented a very good work using sophisticated techniques, such as high resolution electron microscopy and neutron diffraction, where a spinel structure has been clearly identified. The commenter proposed that it should also be important to also more traditional NMC powders to clearly distinguish them from these new high capacity type materials.

Reviewer 3:

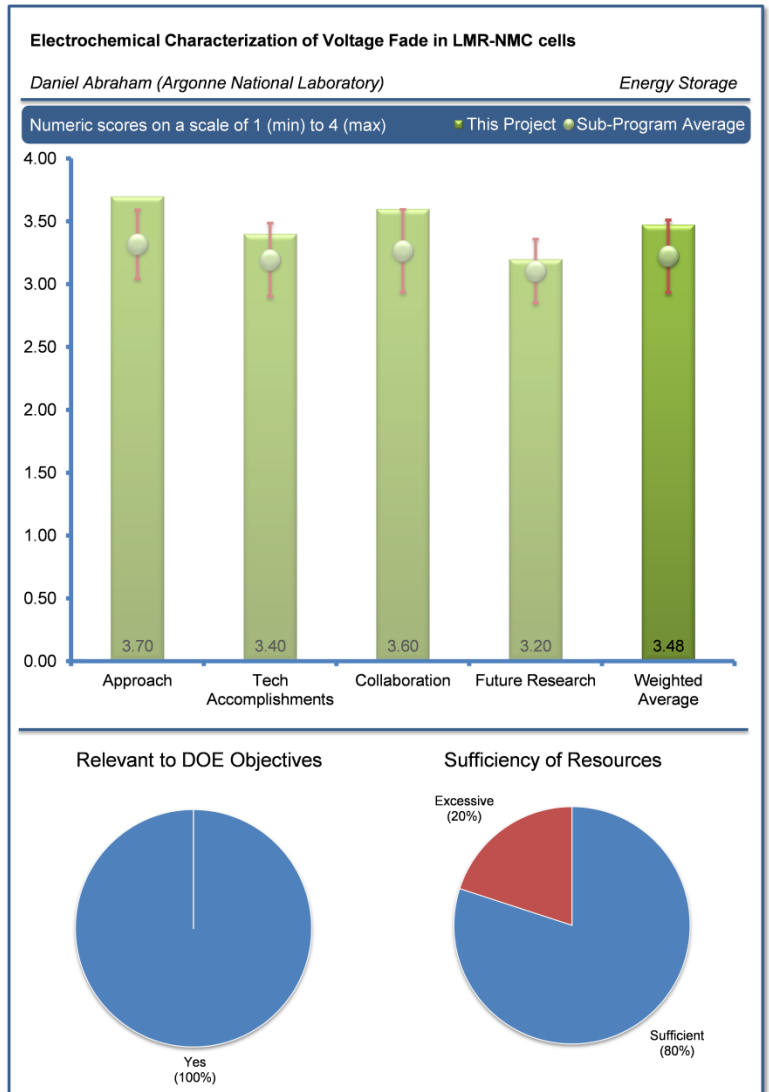
The reviewer highlighted that life is an important barrier for these advanced cells, perhaps the most important at present. As a result, a relevant and standard test is key to unravelling the mystery of why there is fade and droop.

Reviewer 4:

The reviewer described that the approach involved systematic electrochemical methods to provide insight of the voltage fade mechanism. The commenter reinforced that comparison with standard materials and extension to long cycle numbers is most valuable.

Reviewer 5:

The reviewer applauded the excellent use of interrupts and other electrochemical techniques to spot and understand changes in the cell electrodes as these helps to divide and address the different causes of fade separately. In particular, the commenter stated that the electrochemical characterization work was very thorough. The reviewer indicated that the PI used a wide range of techniques and looked



at the effect of many variables on both performance and the electrochemical behavior in great detail. Overall, the reviewer praised the very nice and useful work.

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.

Reviewer 1:

The reviewer stated the accomplishments and progress were very good. The commenter noted that there were some very useful and practical information regarding what can be done to ameliorate the voltage fade, such as decreasing the upper voltage limit during cycling, including a chart provided to show the effect of this on specific energy. The reviewer explained that while the LMR-NMCs cycled to lower voltages are still very attractive, alternatives like NCA (or high voltage NMC if capacity fading can be fixed) appear to be competitive. The reviewer also expressed that it was also good to see neutron diffraction (ORNL) used to detect Li in tetrahedral sites in cycled samples.

Reviewer 2:

The reviewer applauded that the authors have shown tremendous progress. The commenter suggested that it could be that as a byproduct of the author's efforts the battery research community may gain additional insight on the behavior of more traditional cathode powders, and also find some mitigating strategies for the voltage fade phenomena.

Reviewer 3:

The reviewer recognized the significant progress made on what causes the problem. The commenter noted that it was hard to parse out what the researchers did, and what others did, but that is the measure of good collaboration. The reviewer noted that there is sufficient progress to be ready to end soon. The commenter pointed out that it was an important step to separate the impedance from the fade. The commenter suggested that the researchers show that the ex-situ data will be at a lower voltage due to relaxation relative to in-situ work.

Reviewer 4:

The reviewer stated the results were very interesting and clearly showed the potential, and limitations, of the Li-rich NMC materials.

Reviewer 5:

The reviewer recognized the researchers' excellent use of interrupts to show how slowly the materials come to equilibrium (slow transition metal migration), especially at high states of charge. This commenter also noted that the work showing lack of benefit on voltage fade when changing the surface (ALD, coatings etc.) is important negative information that is consistent with the other findings of the team. The reviewer also pointed out that the reference electrode work was also a key element of this program. The project evaluator highlighted the good understanding of the role of the counter-electrode on cell behavior (LTO versus lithium metal versus carbon), but cautioned that they did not see any problems with the system the researchers are using, as they obviously fully understand the implications of the choice of the counter. The commenter mentioned that the researchers clearly showed the effect of charge and discharge voltage limits. Finally, the reviewer simply recognized that a lot of work was done, and applauded the very nice progress.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer affirmed that the deep dive project really was a team effort. This person described that the electrochemical effort was really central to defining the problem and providing guidance to the characterization efforts at ANL. The commenter also described that the project was coordinated with ORNL on neutron diffraction experiments-, one of the few in this program that utilized outside institutions. The commenter suggested that it would be have been nice to see a project like this opened up more to other national labs and universities to avoid the risk of "groupthink."

Reviewer 2:

The reviewer applauded that the project was a true collaboration, with the researchers working with the partners to advance on all fronts. The commenter proposed that the collaboration could only be improved with more collaboration outside the team.

Reviewer 3:

The reviewer acknowledged the strong collaboration with other groups was clearly shown.

Reviewer 4:

The reviewer confirmed the excellent cooperation within the Voltage Fade Team.

Reviewer 5:

The reviewer simply stated that the project included a great team approach.

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.

Reviewer 1:

The reviewer recounted that this deep dive project is ending this year, so the future work is focused on wrapping up loose ends, and providing data to the battery community (presumably in the form of presentations and publications).

Reviewer 2:

The reviewer stated that the future plans are appropriate given that the work is ending. The reviewer thought that it is absolutely critical to show that the protocol, which was legitimately developed without the knowledge gained in the program, does not draw conclusions that would be different if there was not an infinite supply of Li.

Reviewer 3:

The reviewer summarized that the future plans will continue to determine the final capacity, energy density and power capability in the final “stable” configuration. The researchers will extrapolate this, as well as the remaining hysteresis, to the final application in a xEV and define benefits compared to hi-Ni NMC.

Reviewer 4:

The reviewer noted the good future plans. The commenter proposed that, if the researchers have time, they could also look into developing a better understanding of the activation cycles.

Reviewer 5:

The reviewer encouraged the researchers to study additional layered oxides. The commenter suggested that the authors may find some general rules that may help to better understand more traditional cathode powders.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed the research is very relevant to DOE’s objectives of petroleum displacement, since LMR-NMC materials are candidate cathode materials for high-energy batteries needed for vehicle electrification.

Reviewer 2:

The reviewer pointed out that this is based on previous DOE funded work that could make a difference in the battery market, and the present work attacks the current biggest barrier to implementation in the market.

Reviewer 3:

The reviewer described that the project results will help to make available high capacity cathode material in order to increase battery energy density and meet DOE targets on xEV vehicles.

Reviewer 4:

The reviewer simply stated that it is obviously critical to understand the electrochemistry of these electrodes.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer explained that the costs were not broken down by individual investigator efforts for this project. The commenter explained that \$4 million over two years is a more than “healthy” investment to make in the study of materials that are extremely problematic, not just because of the voltage fade issue but because of other issues as well (low tap density, low rate capability, etc.). The reviewer suggested that one could reasonably question if the money would have been better spent on development of other materials and materials discovery and be spread out to other institutions as well. The reviewer would have liked to have seen a more comprehensive comparison of the LMR-NMC materials to other possibilities (high voltage spinel, high capacity stoichiometric NMCs, materials containing two lithium ions per formula unit, etc.). The reviewer also requested the researchers should compare materials not just based on gravimetric capacities, but also densities, rate capabilities, electrode formulations necessary to overcome rate limitations (a high carbon content will compromise energy density), stage of development, projected timeline to commercialization, etc.; only with this information is it possible to make a fair assessment on whether this was money well-spent or not.

Reviewer 2:

The reviewer observed that a lot of work accomplished, so the project was a great use of the funds.

Reviewer 3:

The reviewer could not say, and noted that this information was not provided.

Electrochemical Modeling of LMR-NMC Electrodes: Anthony Burrell (Argonne National Laboratory) - es189

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer explained that system modeling on cells containing LMR-NMC cathodes was carried out using Dualfoil (the Newman program that is used to simulate intercalation in batteries). The commenter noted that this can yield valuable information for well-behaved conventional systems, but the complicated behavior of the LMR-NMC cathodes proved to be very challenging. The reviewer explained that the existence of hysteresis and phase changes means that several time constants need to be used to model the data and experiments need to be slow enough so that equilibrium can be achieved.

Reviewer 2:

The reviewer commented that the electrochemical modeling, coupled with experimental results, validate the results that were presented by the group.

Reviewer 3:

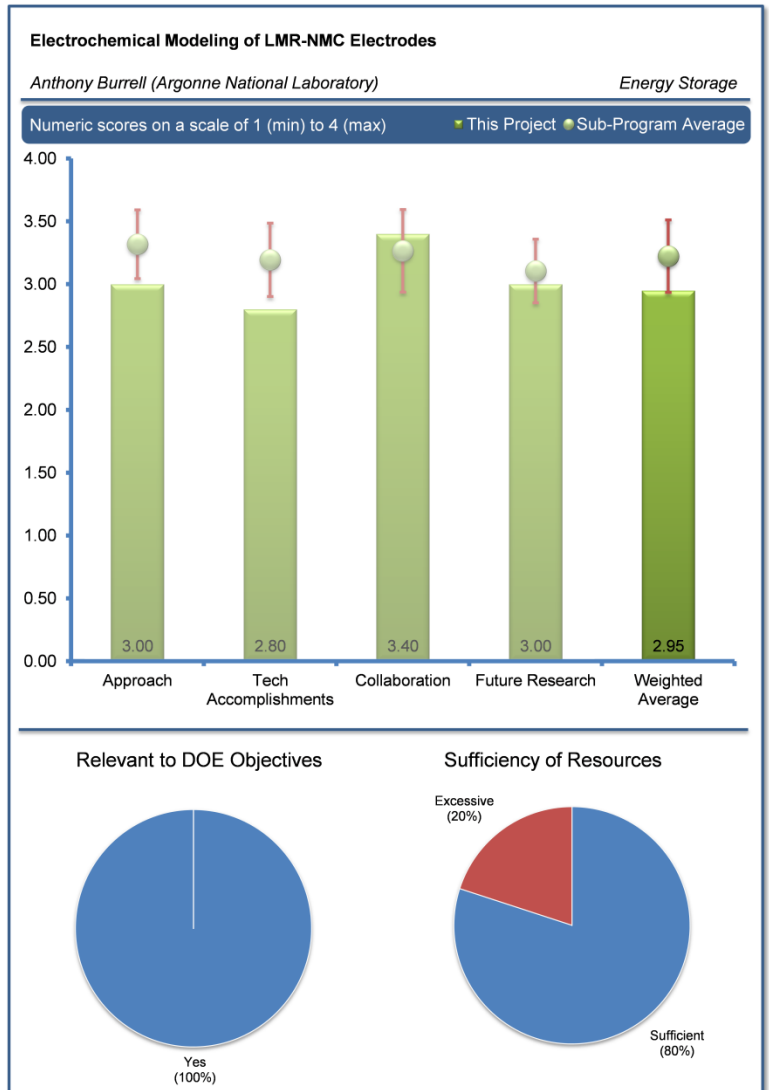
The reviewer noted that the modeling approach is useful, but makes progress only when it is tightly and interactively tied to experimental groups; therefore, being part of this team makes this approach more productive.

Reviewer 4:

The reviewer said that the modeling approach follows standard principles and equations. The commenter explained that the high number of parameters are adjusted by fitting to experimental results. This person suggested that this could be reduced by trying to determine physical parameters in separate experiments.

Reviewer 5:

The reviewer praised the good leveraging of referenced cell work. However, the reviewer said that the approach taken is seems basically a fitting exercise; thus, even if it can fit the data, the reviewer asked what does it really tell us. The commenter proposed that maybe more insight could be gained by modeling the phases separately and linking them to the ab-initio modeling work. The commenter concluded by stating that, as usual, this PI does a nice job of checking for consistency of the models by fitting a variety of cell data on different types of tests.



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.**Reviewer 1:**

The reviewer strongly encouraged exploring additional synthetic routes to produce layered-layered materials with stabilized spinel component. The commenter also strongly encouraged the researchers to investigate mitigating strategies.

Reviewer 2:

The reviewer reported that the results are representing well the fitted experimental data, though the capability to forecast effects has not yet been shown.

Reviewer 3:

The reviewer pointed out that several models were completed and were compared to results in experiments. The commenter noted that there was good agreement to the experiments, though this is fitting and not prediction, so a good agreement is expected. The reviewer concluded by stating that hopefully the approach will be useful in engineering an attack on the fade problem.

Reviewer 4:

The reviewer criticized that the “black box” approach of Dualfoil to modeling this complicated system was somewhat disappointing in the results it yielded. The commenter explained that hysteresis and voltage fade introduced a lot of complexity into this system, which was really developed for simpler dual intercalation systems. The commenter acknowledged that the researcher did indicate that a prediction that current should fall and then rise after long times during a voltage step was confirmed experimentally.

Reviewer 5:

The reviewer reported that the work was able to predict some phenomena that were later observed experimentally, but overall the reviewer questioned the usefulness of this model. With such a complicated material and so many parameters to adjust, the resulting model seems to be largely to be a fitting exercise. The reviewer stated that they look to modeling to explain what is going inside the cell and material. So just fitting data does not do much for this commenter, even though they know people obsess about getting the "fit" right. The reviewer did note that the same model can apparently fit multiple types of test data and this adds to its credibility.

Bottom, line the reviewer thought that this project this is a valiant effort, but the end result was not worth it in their view. While the reviewer reported hating to sound defeatist, maybe this material is just too complex to create a truly useful model of the whole material. The reviewer did, however, think that this work has been useful in highlighting the importance of the cell history that is especially important for this system because it has such long relaxation times before the systems fully recovers on rest. This also indicates that performance testing of this material will likely be a much stronger function of the precise test regime than for other systems. Thus, the project evaluator proposed that a wider array of tests may be required to check for good/bad things that will happen in real-world usage that would otherwise be hidden if one only runs the standard accelerated tests on the cells.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer reported that the researchers were able to give teammates reasons for their observations, and obviously got lots of needed data from them.

Reviewer 2:

The reviewer simply acknowledged the excellent cooperation within the Voltage Fade Team.

Reviewer 3:

This reviewer observed that collaboration seems to be good.

Reviewer 4:

The reviewer explained that this deep dive project was a close collaboration among (mainly) ANL scientists and was clearly a team effort. The reviewer would have liked to have seen more consultation with researchers outside of ANL to avoid falling into the trap of “groupthink.” The commenter reported that the work is being carried out in many groups throughout the world on these materials, and interactions with these researchers would have added valuable perspective.

Reviewer 5:

The reviewer described that the researcher works with electrochemists and cell makers very well to leverage their experimental data. The commenter acknowledged that getting data from referenced cells is critical to their work - and to others in separating out anode and cathode behavior. The commenter stated that the PI can also model these basic electrochemical tests (such as differential capacity plots). The reviewer explained that the PI was able to run the model on real-world tests to predict the actual battery performance seen by the experimenters. The project evaluator explained that modeling work like this also helps highlight to the experimenters/ab-intio modelers what it is that they do not know; this can be very useful in getting them to fill those gaps with their own fundamental experimental/modeling work.

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.

Reviewer 1:

The reviewer simply stated that suitable plans were presented.

Reviewer 2:

The reviewer stated that this deep dive project is ending this year, so the future work is directed towards wrapping up loose ends.

Reviewer 3:

The team effort demonstrated during this work seems to be continuing as shown by the authors during their presentation. This reviewer suggested that the authors should explain in more detail the assumptions involved in the models and calculations.

Reviewer 4:

The reviewer suggested that the model should be tested by forecasts of certain effects (at fixed data set) to be checked afterwards by experiments. The commenter also requested that the researchers try to determine as many physical parameters as possible by dedicated measurement of those parameters.

Reviewer 5:

The reviewer explained that this approach has to lump many variables together for the different phases. The reviewer suggested that maybe more insight could be gained by modeling the phases separately and linking them to the ab-intio modeling work rather than data from actual cells (or maybe to cell data for cells using the component phases if that were possible). The reviewer asked whether there any value/insight that can be gleaned from the parameters used to fit the model to the data. If not, the commenter stated that it is hard for them to really see that there is much value in this work.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer reported the work is very relevant to DOE’s objectives of petroleum displacement since LMR-NMC materials are candidate cathode materials for high-energy batteries needed for vehicle electrification.

Reviewer 2:

The reviewer indicated that the layered material is a DOE-funded advancement, so this project enhances past work. The commenter also explained that the material is also a step forward that is just outside of making a real commercial impact due to droop and fade, and so this work is very much on point for putting more EVs and PHEVs on the road.

Reviewer 3:

The reviewer described that the project is focused on helping to make available high capacity cathode material in order to increase battery energy density and meet DOE targets on xEV vehicles.

Reviewer 4:

The reviewer stated that the project supports experimentalists to study "hot" cathode material, but the fitting nature of the model makes the reviewer question its utility.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer explained that the costs were not broken down by individual investigator efforts for this project. The commenter explained that \$4 million over two years is a more than "healthy" investment to make in the study of materials that are extremely problematic, not just because of the voltage fade issue but because of other issues as well (low tap density, low rate capability, etc.). The reviewer suggested that one could reasonably question if the money would have been better spent on development of other materials and materials discovery and be spread out to other institutions as well. The reviewer would have liked to have seen a more comprehensive comparison of the LMR-NMC materials to other possibilities (high voltage spinel, high capacity stoichiometric NMCs, materials containing two lithium ions per formula unit, etc.). The reviewer also requested the researchers should compare materials not just based on gravimetric capacities, but also densities, rate capabilities, electrode formulations necessary to overcome rate limitations (a high carbon content will compromise energy density), stage of development, projected timeline to commercialization, etc.; only with this information is it possible to make a fair assessment on whether this was money well-spent or not.

Reviewer 2:

The reviewer could not really say, and noted that this information was not provided.

Synthetic Approaches to Correcting Voltage Fade in LMR-NMC: Christopher Johnson (Argonne National Laboratory) - es190

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer noted an excellent and comprehensive study. The reviewer added that it was interesting to see that the authors did not hesitate in taking a decision about the coating approach on voltage fade.

Reviewer 2:

The reviewer commended the good multi-tool, multi-discipline approach. The commenter acknowledged the rigor of maintaining same amount of Li, or fixing the rest of the structure as cations are changed, is a very good to answer this problem.

Reviewer 3:

The reviewer agreed that a good systematic experimental approach was used. The reviewer indicated that the link to theory/modeling to direct experiments were stated, but could not be seen.

Reviewer 4:

The reviewer recognized the excellent synthetic approaches and link to modeling efforts.

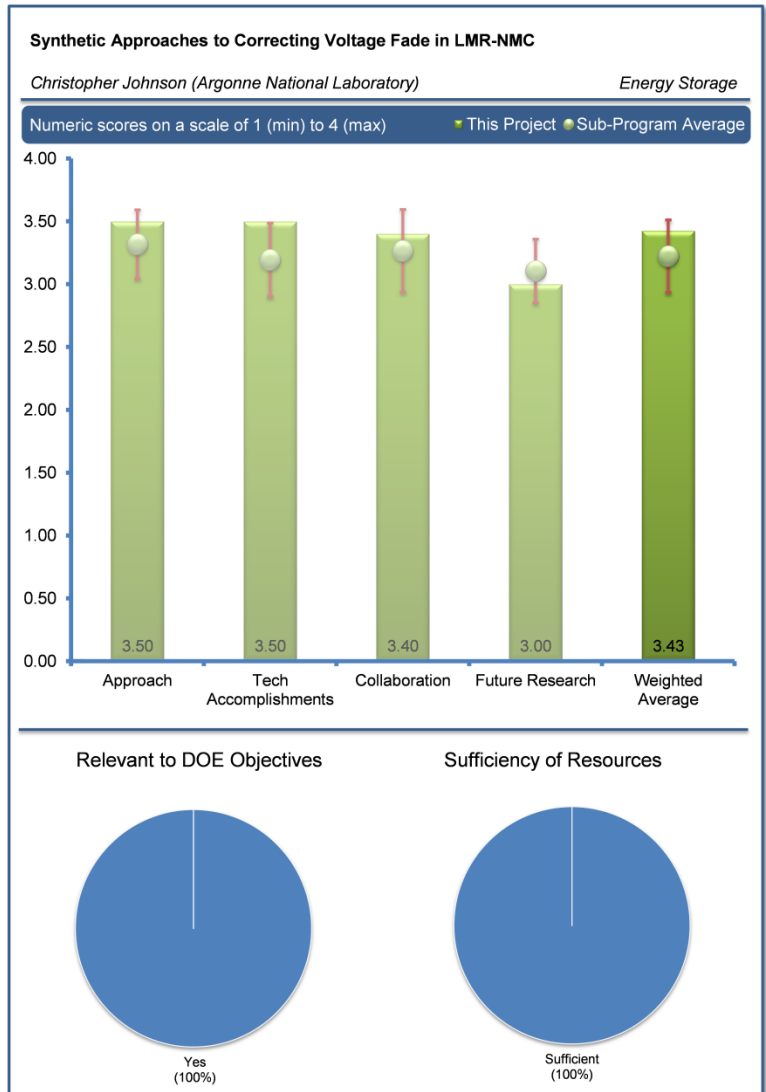
Reviewer 5:

The reviewer commented that the approach is quite broad and well-conceived. The only problem the reviewer reported seeing is the limitation of elemental substitution to the trivalent component (substituting Al, Ga, and Fe for Co). As the PI recognized, substitution of Ru for Mn has a major effect on the voltage fade. The commenter suggested broadening the search for substituents to those involving Mn with other tetravalent elements and in trivalent/pentavalent 1:1 combinations. The reviewer mentioned that work by Tarascon has suggested that Sn-Ru mixtures have a major effect on reducing or eliminating voltage fade in similar lithium-rich composite materials, which gives emphasis to this type of study.

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.

Reviewer 1:

The reviewer pointed out that although major effects to solve voltage fade have not resulted from the work so far, a number of relevant studies have eliminated factors as having any important effect on voltage fade. This includes the effect of synthesis method, synthesis conditions, relative compositions among Li, Ni, Mn, and Co. The correlation of the ratio of Co/Mn as causing an increase in voltage



fade was not convincing to the reviewer, as it appeared that the result is within the range of error. The reviewer also suggested that a regression analysis of the data be carried out to test the reliability of this important conclusion.

Reviewer 2:

The reviewer stated that the PI clearly explained the issue involved with voltage fade. The reviewer opined that the increased understanding of this phenomenon should be able to push forward mitigation strategies to the voltage fade issue. New synthetic strategies and better understanding of the cations movement while cycling these materials should be continued.

Reviewer 3:

The reviewer summarized that the project is pulling many threads of research together the main causes seem to be largely defined. The commenter acknowledged that this required a lot of work to complete like coatings, doping, and synthesis investigations. The reviewer remarked that the sol gel method was a very good choice of ways to look at the ion species impact.

Reviewer 4:

The reviewer recognized the extensive and meaningful results that clearly showed that voltage fade is a reproducible and imminent feature of the structure and only depends a little on the synthesis route or specific composition.

Reviewer 5:

The reviewer commended the nice synthetic work. The commenter explained that the researchers looked at quite a wide variety of synthetic methods, and the lack of affect does support their contention that the problem is innate to the material itself. While this work shows that surface coatings do not affect the voltage fade, the commenter indicated that it does show promise for reducing some of the other causes of fade. The reviewer reported that while the researcher acknowledged the DOE's goals of thousands of cycles for a PHEV battery, it seems to the reviewer that some of the approaches to the other aspects of fade could realize cycle life that was at least in the 100-300 cycles range. The commenter suggested that this would be good enough for many consumer applications, especially as each cycle would be longer than that for a typical Li-ion cell. Thus, the commenter suggested that establishing what the best cycle life could be using these approaches may be enough to start it being commercialized. Apart from the monetary aspects, the reviewer indicated that the attention this would then get from the cell makers would greatly add to the number of researchers working to optimize the material. By leveraging the large staff of the commercial enterprises, this might actually be the best way to fix the problems for longer cycling that the DOE needs.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer agreed there was excellent cooperation within the Voltage Fade Team.

Reviewer 2:

This reviewer asserted that the authors are clearly coordinating their research efforts.

Reviewer 3:

The reviewer commended that the collaboration was excellent in team, but not much outside team. The reviewer said that was OK and the level of cooperation across the groups in such a huge team was pretty impressive.

Reviewer 4:

The reviewer affirmed that the collaboration among the ANL workers is exemplary. The reviewer felt, however, that additional collaboration with battery manufacturers (especially in the EV space) would be very useful to include to focus the future work on what would be acceptable performance in the various types of xEVs for this potentially valuable material. The reviewer acknowledged that this might move the program to include additional studies to truly evaluate the LMRNMC family in actual application tests of interest to manufacturers. The commenter offered that this is especially valuable in a large team effort such as this to accelerate the implementation of the material in actual cells as the work continues.

Reviewer 5:

The reviewer stated that there was a good link to some modeling efforts, but criticized that the modeling at Berkeley by Persson (Project Number es091), where they largely seem to discount the dumbbell mechanism, seems to have been ignored.

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.

Reviewer 1:

The reviewer offered that if the voltage fade issue cannot be easily resolved, that developing mitigating strategies should be strongly encouraged. The reviewer expressed that these type of powders are too important for the future of high capacity Li-ion cells.

Reviewer 2:

The reviewer agreed that it was too strong to conclude that a fix is unattainable. The commenter suggested that the focus needs to be how to “fix” the problems identified here, so the fade is eliminated.

Reviewer 3:

The reviewer criticized that some of the proposed next steps are not target-oriented, as shown by some other groups. The commenter suggested that a new focus could be to find a synthesis route to produce the material in the structural configuration, which was found to be the stable one (after several hundred cycles).

Reviewer 4:

The reviewer agreed that it was critical to look at doping with Ru, Sn, etc. that Tarascon has apparently published. The commenter was glad to see this is planned, but emphasized that reproducing, and even understanding better, Tarascon's work needs to be a top priority for this project and especially this PI.

Reviewer 5:

The reviewer stated that they would like to see an expansion of the substitution work to tetravalent ions. The reviewer requested seeing a better validation of the spinel component in the LLS materials as suggested by the PI.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed the project is highly relevant.

Reviewer 2:

The reviewer commented that the DOE work will be enabled and the energy of cells could be increased over today's normal cell if this problem is solved.

Reviewer 3:

The reviewer stated that the project will help to make available high capacity cathode material in order to increase battery energy density and meet DOE targets on xEV vehicles.

Reviewer 4:

The reviewer agreed that the project is very important in establishing what does, and equally important what does not, help voltage fade.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer indicated that it was hard to say, and noted that this information was not given.

Atomic-Scale Models of LMR-NMC Materials: Hakim Iddir (Argonne National Laboratory) - es193

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer explained that a first principles modeling of materials was used to understand their behavior. The commenter noted that although there are some limitations to using density function theory (DFT) GGA+U on materials with mixed conductivities, when done judiciously, useful insights can be obtained. The project evaluator state that focusing on a composite Li_2MnO_3 -LCO material is closer to the real-world LMR-NMC material than pure Li_2MnO_3 (which behaves much differently), but it would have perhaps been more relevant to look at a Ni-containing composite instead, since that is what is being proposed for use.

Reviewer 2:

The reviewer reported that the approach followed by the authors, where theoretical calculations were coupled with experimental results, was excellent and of high quality.

Reviewer 3:

The reviewer stated that the researchers used a good approach that was a key to the team's success.

Reviewer 4:

The reviewer remarked that it was important approach to couple the experimental results with the first principle simulations. The commenter mentioned that regarding oxygen vacancies model was calibrated to experiment. The reviewer asked if it was possible to simulate the kinetics of the oxygen release.

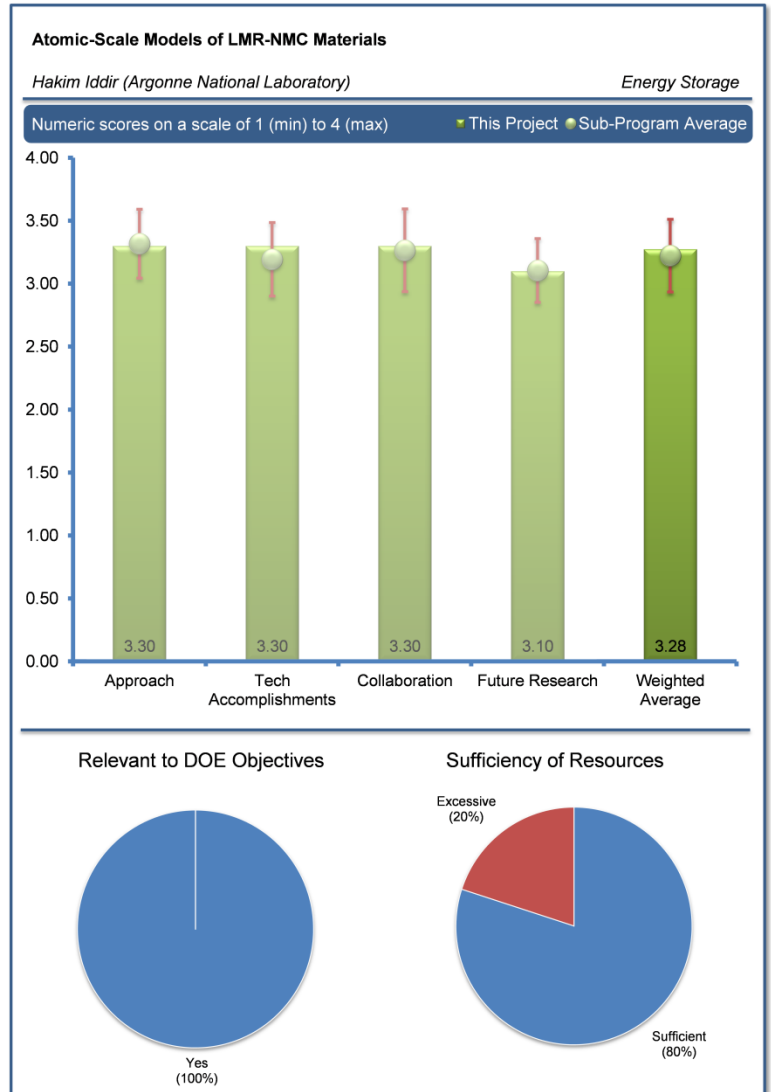
Reviewer 5:

The reviewer praised the good use of modeling to understand the important aspects of this complex material and the good comparison with NMR and X-Ray Absorption Near Edge Structure (XANES) studies. The commenter, however, was concerned about the apparent disconnect with similar modeling at Berkeley on Li_2MnO_3 phase.

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.

Reviewer 1:

The reviewer reported that calculations indicated that there is a tendency for phase separation to occur in the Li_2MnO_3 -LCO system, with domains in ribbons. The commenter explained that Co is oxidized first, which is perhaps not too surprising (one might expect Ni



to oxidize first in an LMR-NMC, however, so this is something different about the chosen system). One surprising result the reviewer noted was the prediction of tetrahedral Mn^{5+} as an intermediate during the cycling. Mn^{5+} is somewhat unstable and may easily disproportionate to Mn^{7+} and Mn^{3+} or Mn^{4+} (particularly if an acidic component is present in the electrolytic solution). The reviewer remarked that it would have been nice to confirm or deny this experimentally, perhaps by using some kind of optical spectroscopy.

Reviewer 2:

The reviewer stated that the theoretical calculations provided by the authors showed that the tetrahedral site for Mn is favored by 0.21 eV over the octahedral site, and they mentioned that this difference is the driving force behind Mn migration. The reviewer asked whether there is any qualitative rule that can explain that trend. The commenter suggested better overlap between Mn and oxygen atoms and/or less repulsion between Mn cation with other metal cations.

Reviewer 3:

The reviewer mentioned that it was useful to know that thermodynamics would drive phase segregation. The commenter stated that the indication of vacancies and Mn movement interaction points to the mechanism in experiments and underpins it with the needed energetics to have confidence it is the mechanism. The reviewer also stated that the long range order in Li interface on long anneal was then seen in experiment.

Reviewer 4:

The reviewer reported that the model has been fully-implemented and the delivered results are showing accordance to the experimental findings.

Reviewer 5:

The reviewer commented that the ability to predict NMR and other experimental data is very important in adding validity to their modeling work, but more importantly it enables the team to really understand the experimental data and figure out what is going on with this very complex cathode material.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer commented that this deep dive project was a close collaboration among (mainly) ANL scientists, but was clearly a team effort. The reviewer would have liked to have seen more consultation with researchers outside of ANL to avoid falling into the trap of “groupthink.” The reviewer acknowledged that work is being carried out in many groups throughout the world on these materials, and interactions with these researchers would have added valuable perspective.

Reviewer 2:

The reviewer simply noted the good and fruitful collaboration with experimentalists.

Reviewer 3:

The reviewer commented that, as with partners, the project is a well-integrated collaboration among many partners.

Reviewer 4:

The reviewer acknowledged the excellent cooperation within the Voltage Fade Team.

Reviewer 5:

The reviewer agreed that, in general, the collaboration seems to be excellent; describing that the researchers are working with NMR, XANES studies, etc. However, the reviewer saw an apparent disconnect and maybe even a fundamental disagreement with the modeling work at Berkeley by Persson (Project Number es091). The reviewer stated that if there is a disagreement between the groups, then that is fine, but resolve it as a team using science, logic, and data. The reviewer suggested that maybe they were wrong, but they got the distinct impression that a “Not Invented Here” syndrome may be in play at the ANL team.

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.

Reviewer 1:

The reviewer simply stated the future plans were adequate.

Reviewer 2:

The reviewer explained that this deep dive project is ending this year, so the future work is directed towards wrapping up loose ends.

Reviewer 3:

The reviewer reported that the theoretical calculations suggested that Mn migration as the main problem with this type of powders. The commenter proposed that it should be of great interest to study that mechanism further, so solutions or partial mitigation strategies can be proposed. This reviewer noted that it could be of great interest if, in the future, the authors qualitatively explain why, or which, is the driving force behind the generation of oxygen vacancies. The reviewer explained that a better understanding of its mechanism may open the door to new mitigation strategies for the voltage fade issue.

Reviewer 4:

The reviewer agreed that the plans are okay, but the reviewer wondered whether the researchers could model the effect of Ru and Sn doping that Tarascon has reported reduces voltage fade.

Reviewer 5:

The reviewer asked whether there was a possibility to extend the model to other compositions or dopants. The commenter also asked whether there was the possibility to identify the/a final 'stable' configuration after cycling as shown by experimental groups.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed that the project was very relevant to DOE's objectives of petroleum displacement since LMR-NMC materials are candidate cathode materials for high-energy batteries needed for vehicle electrification.

Reviewer 2:

The reviewer commented that the project would make vehicles or MP3s go further or longer. The reviewer also mentioned that the project supports DOE work that created this material in the first place.

Reviewer 3:

The reviewer agreed that the project will help to make available high capacity cathode material in order to increase battery energy density and meet DOE targets on xEV vehicles.

Reviewer 4:

The reviewer stated that fundamental modeling like this can provide key insights to these complex and very important material that cannot be attained experimentally.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer explained that the costs were not broken down by individual investigator efforts for this project. The commenter explained that \$4 million over two years is a more than "healthy" investment to make in the study of materials that are extremely problematic, not just because of the voltage fade issue but because of other issues as well (low tap density, low rate capability, etc.). The reviewer suggested that one could reasonably question if the money would have been better spent on development of other materials and materials discovery and be spread out to other institutions as well. The reviewer would have liked to have seen a more comprehensive comparison

of the LMR-NMC materials to other possibilities (high voltage spinel, high capacity stoichiometric NMCs, materials containing two lithium ions per formula unit, etc.). The reviewer also requested the researchers should compare materials not just based on gravimetric capacities, but also densities, rate capabilities, electrode formulations necessary to overcome rate limitations (a high carbon content will compromise energy density), stage of development, projected timeline to commercialization, etc.; only with this information is it possible to make a fair assessment on whether this was money well-spent or not.

Reviewer 2:

The reviewer could not say, and noted that this information was not provided.

Understanding Structural Changes in LMR-NMC Materials: Jason Croy (Argonne National Laboratory) - es194

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer described that X-Ray Absorption Spectroscopy (XAFS) was used to investigate local structures of LMR-NMC cathodes. The reviewer agreed that this was a good method for detecting changes in local ordering in transition metals containing battery materials as a function of composition, state-of-charge, and cycle number, although the commenter indicated that the results were somewhat hampered by the inability to directly observe Li-ions due to their near X-ray transparency. For this reason, the reviewer suggested that the technique is best used in conjunction with other techniques (e.g., neutron diffraction, NMR, and etc.) to understand the full picture, as was done in this project.

Reviewer 2:

The reviewer expressed that this is an important effort that clarifies some of the problems associated with voltage fade. The reviewer inquired about the existence of any qualitative rule such as the ones used in organometallic chemistry that the authors can propose to explain the generation of oxygen vacancies.

Reviewer 3:

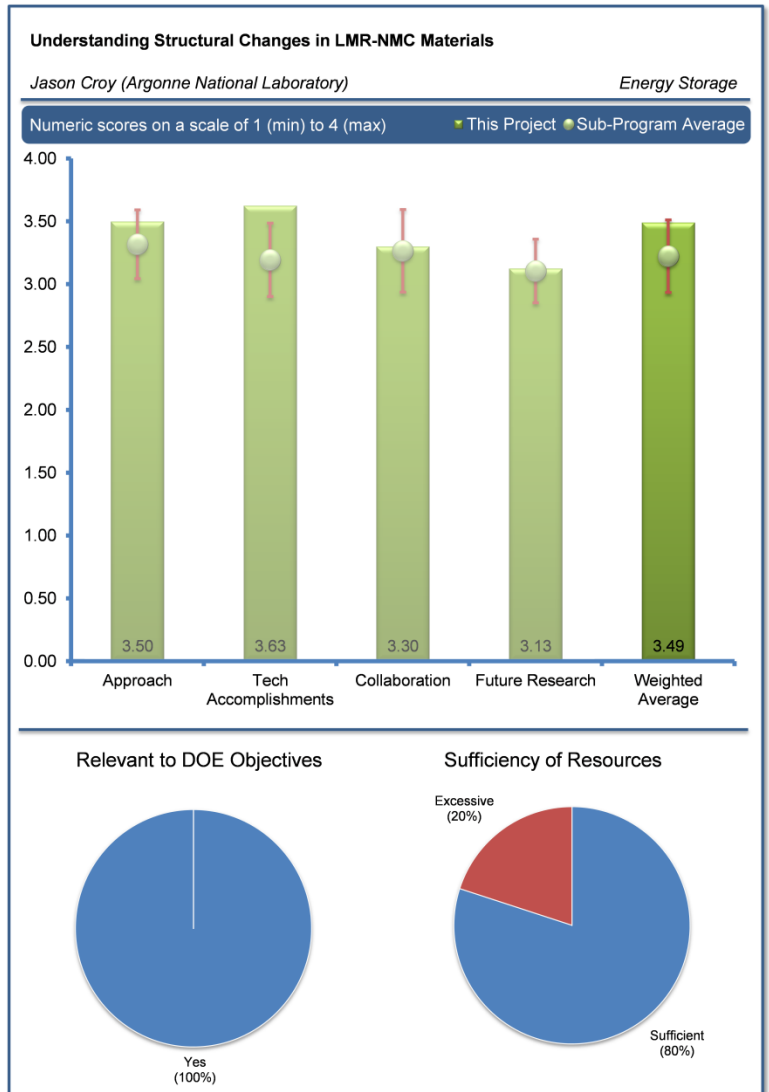
The reviewer applauded the nice technique used to look at the structure. The commenter pointed out that the researchers went past the structure to the energetics, which is the main problem, so this was a good way to study the part of the scope they were assigned.

Reviewer 4:

The reviewer praised the excellent analytical approach that was used to reveal the voltage fade mechanisms.

Reviewer 5:

The reviewer noted the good combination of modeling, electrochemistry, XANES, and EXAFS diffraction analysis.



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.**Reviewer 1:**

The reviewer expressed that this work, which reflects efforts by both this PI and other team members, has shown excellent insight as to what is going on inside this complex cathode material. Overall, the commenter said that this has greatly boosted the battery research community's understanding and appears to have largely answered the key questions.

Reviewer 2:

The reviewer acknowledged that important findings such as the trapped Mn species in tetrahedral sites. The commenter stated that this type of information is critical so mitigating strategies can be developed. This reviewer observed good interaction with other groups that complement the project team's results. It could be of interest to better explain the uncertainty involved in the fittings of the EXAFS spectra.

Reviewer 3:

The reviewer reported that the researchers showed that distortion of matrix and Mn^{3+} occurs after cycling and also that the structure and oxidation state vary on charge and discharge at same voltage.

Reviewer 4:

The reviewer reported that substantial insight in structural changes during activation and first cycles have been elaborated.

Reviewer 5:

The reviewer explained that XAS, when used in conjunction with other techniques, can provide useful information about local structures and metal oxidation states. In pristine materials, there is evidence of segregation of Mn into Mn-rich regions. This is consistent with interpretation of the structure as being a "layered-layered" composite, but also with a solid solution having a flower pattern arrangement of cations in the transition metal layers. The commenter noted that different rates of cooling during synthesis did not result in substantial differences in XAFS patterns for one particular material with unspecified X, suggesting perhaps that it is a composite regardless of the cooling rate. The project evaluator also indicated that the transmission electron microscope analysis also seemed to show that it is a composite, but solid solutions with planar defects can look like a mixture of rhombohedral and monoclinic materials in some views, so this was not conclusive either. The reviewer agreed that it is certainly possible that some compositions are composites (e.g., Toda HE5050) and others are solid solutions, so it was best not to assume that all LMR-NMCs are the same. It seemed to this commenter that much of the XAFS data can be interpreted at least two different ways (e.g., Li_2MnO_3 in $0.5Li_2MnO_3 \cdot 0.5LiNi_{0.5}Mn_{0.5}O_2$ looks different from pure Li_2MnO_3 ; but the reviewer asked whether this was because it was influenced by the rhombohedral component or because it was not really a separate phase.)

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer explained that this deep dive project was a close collaboration among (mainly) ANL scientists, and was clearly a team effort. The reviewer would have liked to have seen more consultation with researchers outside of ANL to avoid falling into the trap of "groupthink." The commenter noted that work is being carried out in many groups throughout the world on these materials, and interactions with these researchers would have added valuable perspective.

Reviewer 2:

The reviewer described that, as with others in this team, great interchange and true collaboration was achieved in the team.

Reviewer 3:

The reviewer recognized the excellent cooperation within the Voltage Fade Team.

Reviewer 4:

The reviewer noted that this work seems to show good coordination and interaction with other groups and laboratories.

Reviewer 5:

The reviewer noted the excellent collaboration with experimentalists. The biggest concern the reviewer had was the apparent lack of collaboration with, and ignoring the modeling efforts at, Berkeley by Persson (Project number es091). The commenter asserted that the researchers' work suggests that the dumbbell model of Mn migration is incorrect, but the dumbbell model is the crux of the mechanism portrayed in this work. The reviewer explained that it is fine if there is a disagreement, but resolve it as a team using science, logic, and data.

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.

Reviewer 1:

The reviewer noted that this deep dive project is ending this year, but some fairly comprehensive future work is planned, rather than just wrapping up the loose ends. This suggested to the commenter that work will continue on the LMR-NMC system in another context (a different project, for example).

Reviewer 2:

The reviewer suggested that studies to increase the cycle numbers might be of interest to follow behavior towards the 'stabilization' of structure (e.g., as shown by Abraham).

Reviewer 3:

The reviewer stated that it was good that the researchers are looking at the activation cycles. The reviewer indicated that they want to see the apparent disconnect between Berkeley and ANL resolved.

Reviewer 4:

The reviewer strongly encouraged the researchers to explore additional synthetic routes to produce layered-layered materials with stabilized spinel component; developing mitigating strategies were also strongly encouraged.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer agreed that the project is very relevant to DOE's objectives of petroleum displacement, since LMR-NMC materials are candidate cathode materials for high-energy batteries needed for vehicle electrification.

Reviewer 2:

The reviewer asserted that the project is needed to make a DOE-funded breakthrough material viable. The commenter also observed that the project would help with driving range for vehicles if it succeeds in fixing the voltage fade issue.

Reviewer 3:

The reviewer stated that the work helps to make available high capacity cathode material in order to increase battery energy density and meet DOE targets on xEV vehicles.

Reviewer 4:

The reviewer commended that the project has addressed, and largely resolved, the key issues in understanding the LLC material which is critical to this program.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer explained that the costs were not broken down by individual investigator efforts for this project. The commenter explained that \$4 million over two years is a more than "healthy" investment to make in the study of materials that are extremely problematic, not

just because of the voltage fade issue but because of other issues as well (low tap density, low rate capability, etc.). The reviewer suggested that one could reasonably question if the money would have been better spent on development of other materials and materials discovery and be spread out to other institutions as well. The reviewer would have liked to have seen a more comprehensive comparison of the LMR-NMC materials to other possibilities (high voltage spinel, high capacity stoichiometric NMCs, materials containing two lithium ions per formula unit, etc.). The reviewer also requested the researchers should compare materials not just based on gravimetric capacities, but also densities, rate capabilities, electrode formulations necessary to overcome rate limitations (a high carbon content will compromise energy density), stage of development, projected timeline to commercialization, etc.; only with this information is it possible to make a fair assessment on whether this was money well-spent or not.

Reviewer 2:

The reviewer could not say, and noted that this information was not provided.

Significant Enhancement of Computational Efficiency in Nonlinear Multiscale Battery Model for Computer Aided Engineering: Gi-Heon Kim (National Renewable Energy Laboratory) - es197

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer asserted that the presentation would have been significantly improved by the presenter not reading the text written on the slide; it would also be improved with less text. The commenter explained that the model seems to be essential to previous and related efforts by others (e.g., companies, national labs, and academia).

Reviewer 2:

The reviewer reported that this project is developing a Multi-Scale Multi-Domain (MSMD) model which will link battery physics across varied length and time scales. The commenter explained that the battery geometry will be resolved into three coupled computational domains to achieve high computational efficiency with a flexible and expandable modularized framework. The project goals include a greatly reduced computational load and the ability to resolve complex transport and kinetics which are often nonlinear interactions.

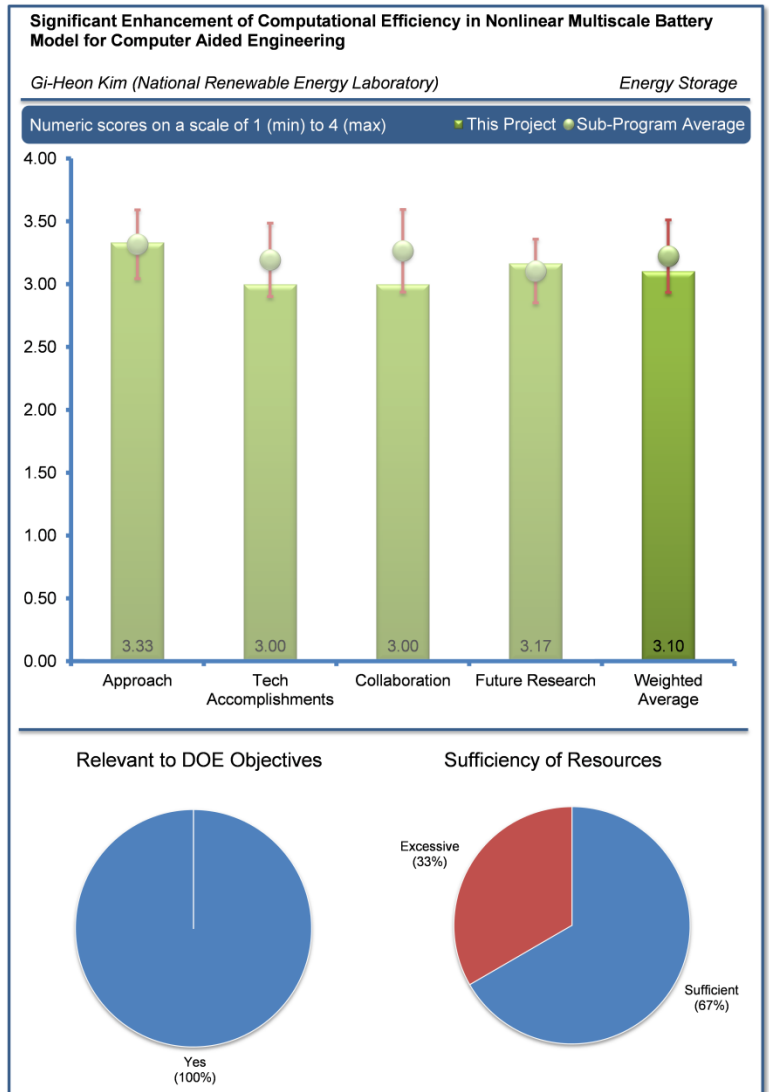
Reviewer 3:

It seemed to the reviewer to be a good approach to link battery physics at different length and time scales to eliminate some of the nested iterations to reduce computation time without compromising accuracy. The commenter noted that adaptive and nonlinear ROM were proposed to improve the accuracy with faster computation time, but explained that not enough details were provided to understand these modified ROMs.

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.

Reviewer 1:

The reviewer stated that the researchers seemed to have made great progress, given that the project was only 25% completed. The commenter recognized that a 100 faster computation speed was claimed and the voltage profile seemed to match between the measured and simulation data. The reviewer proposed that more validation data should be provided to show progress toward mitigating instabilities caused by nonlinearity.



Reviewer 2:

The reviewer noted that the project is relatively new. The goals for the project were outlined: ROMs have limitations. The commenter described that a new technique using low-order which are adaptive to system evolution, are to be developed. In addition, the reviewer reported that a new ROM that does not fail under severe nonlinear conditions (with speeds comparable to current ROMs) will be designed. Multiple options of modular component models for various subsystems will also be constructed to avoid current limitations for various battery designs, environments and operating conditions. It was not clear to the reviewer how far the work on these topics has progressed. The project evaluator described that the presentation focused on the newly developed GH-MSMD framework that has been implemented, which links the particle domain model into the electrode domain model. The commenter observed that this framework removes the nested iterations, but retains the modular architecture thus achieving a significant enhancement in computational speed. Some data was made available regarding potential output/applications from the project - this included insight into how active electrode material particles respond under differing driving cycles (HEV versus PHEV). The reviewer recognized that the project is relatively new, but suggested that early validation with more developed models and experimental data would be welcome to verify that the new implementations do not skew the information obtained.

Reviewer 3:

The reviewer indicated that the presenter did not spend enough time presenting this. The commenter described that the results were on battery simulations, and did not address the computational efficiency improvements which are the main focus of the project. The reviewer criticized that the reviewer only noticed one number on one slide (i.e., 100 times improvement in computational time), but no discussion of what the computational efficiency was due to was provided.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer agreed that there seemed to be good collaboration with specific roles described for each team member.

Reviewer 2:

The reviewer stated that this project is led by NREL in partnership with ANSYS. The team of researchers will integrate the outcome models of ANSYS's battery simulation platform by providing ANSYS software engineering in support of the NREL researchers. The commenter stated that previous collaborations between these partners suggest that a strong fusion of their respective talents will be brought to the project tasks. The reviewer suggested that perhaps discussions with the teams developing the CAD tools for CAEBAT (i.e., CD-adapco, EC Power, and GM-ANSYS) would be welcome to ensure that the evolution of the computational models is understood by all and that feedback can be obtained as the work is done or beforehand.

Reviewer 3:

The reviewer suggested that it would be nice to have more academic contributions.

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.

Reviewer 1:

The reviewer explained that the future research will extend the GH-MSMD nonlinear multiscale framework to include cell domain models and subscale domain models. A Discrete Empirical Interpolation Method for the representation of the nonlinear functions will also be added to aid in retaining the use of ROMs. The commenter also indicated that metrics will be developed to evaluate the relative enhancement of the models and the framework will be incorporated into the ANSYS CAEBAT framework and the Open Architecture Software. Finally, the reviewer stated that validation of the model codes against the baseline full-order (slower) models will be done. The reviewer summarized that the proposed future work is well-aligned with the project's milestones.

Reviewer 2:

The reviewer proposed that the researchers should focus more on modeling of aging to show that the instabilities caused by nonlinearity can be mitigated with their approach, while not compromising accuracy.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer mentioned that battery physics-based computational models are often hampered by excessive computational expense due to transport and kinetic interactions which are often nonlinear; this project seeks to address these challenges.

Reviewer 2:

The reviewer agreed that this is a worthwhile effort to reduce the computation time without compromising accuracy. If successful, the reviewer said it should make the use of battery modeling more mainstream among battery engineers/scientists.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that the project should enable collaborations with universities at the \$1.2 MM level.

Reviewer 2:

The reviewer indicated that no information about the resource availability was provided, so it was assumed that sufficient resources are available for the project's milestones.

Coupled Hierarchical Models for Thermal, Mechanical, Electrical and Electrochemical Processes: Harry Moffat (Sandia National Laboratories) - es198

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer liked the use of CANTERA to enable the incorporation of the various physics of kinetically-controlled phenomena.

Reviewer 2:

The reviewer described that the project will incorporate thermodynamic and kinetic properties from the literature into a CANTERA-based framework for cell-level chemistry/transport. The commenter also pointed out that models from Sandia National Laboratories' (SNL) Thermal Battery Program will be added to the CAEBAT architecture. Partial saturation and solid mechanics models will be added (to address gasification and stress-induced degradation). SEI models will be constructed that predict experimental autocatalytic temperature behavior. Microstructure calculations will be up-scaled to the macrohomogeneous scale. Finally, new models will be developed for thermal runaway processes. Unfortunately, reviewer criticized that the presenter did not sound overly confident in the proposed approach; it seems that significant challenges may complicate the work ahead.

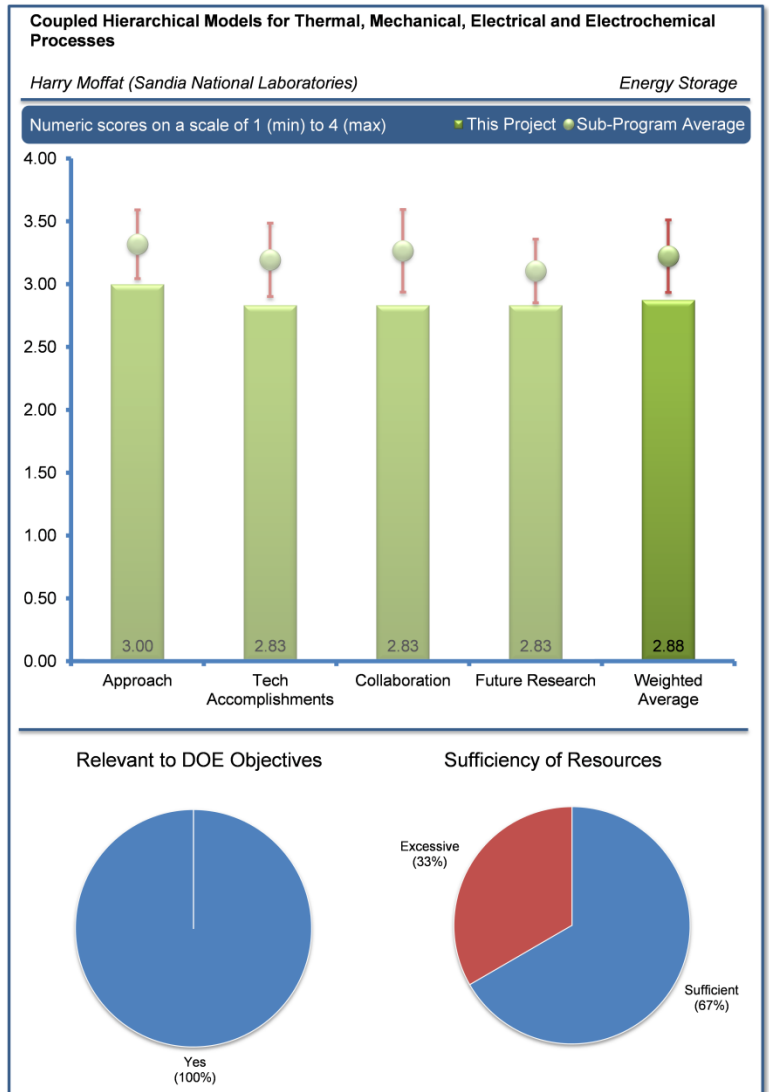
Reviewer 3:

The reviewer described that the researchers proposed to simulate thermal runaways using predictive mechanisms derived from coupled electrochemical and thermal models. The commenter acknowledged that the researchers also had good idea to add side reactions and gas generations in their CANTERA electrochemical model. However, the commenter remarked that this might be very challenging since no one has a complete understanding of all the side reactions and gas generation reactions. The reviewer noted that the researchers' intent to use empirical exchange current and to use look-up table for their scale-up electrochemical heating seemed to contradict their mechanism based.

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.

Reviewer 1:

The reviewer commented that later this year a go/no-go point will be the duplication of existing capabilities (from NTG and Dualfoil) with the CANTERA/1DElectrode framework within the CAEBAT architecture (incorporating an electrode object into CAEBAT). The



commenter reported that accomplishments noted include: an electrode evolution model, the understanding of numerical issues associated with the work, and heat release capability. The reviewer explained that slides were provided for a collaborator at the Colorado School of Mines who is focused on providing more realistic electrode microstructure models rather than the simple spherical models of active material particles currently used. It was unclear to this person if the work shown is from some previous work, or if it was done as part of the present project. The reviewer summarized that for these more realistic models, pre-computed look-up tables will be used facilitate the determination of heat release.

Reviewer 2:

The reviewer explained that since this project was just kicked off, there was limited accomplishment, but the researchers need to show more thermal distribution data as a function of discharge rates.

Reviewer 3:

The reviewer said that not much progress since the project just started.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer noted that the project is led by SNL with ORNL providing the CAEBAT Open Architecture Software and a researcher at the Colorado School of Mines providing upscaling of the pore-level models. Perhaps discussions with the teams developing the CAD tools for CAEBAT (i.e., CD-adapco, EC Power and GM-ANSYS) would be welcome to ensure that the evolution of the computational model is understood by all and that feedback can be obtained as the work is done or beforehand. Direct discussions with OEMs about their experience with thermal runaway and their desired output from a new model would also perhaps be fruitful.

Reviewer 2:

The reviewer observed good collaboration with various teams and that specific roles were described.

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.**Reviewer 1:**

The reviewer explained that the future research includes implementation of solid mechanics, partial saturation, and pressurization models to enable multi-phase capability followed by the addition of SEI models, and a demonstration of the model's capabilities. The commenter highlighted that direct validation (preferably including blind evaluations) of the framework is necessary; otherwise the resulting framework will have little utility.

Reviewer 2:

The reviewer stated that the future work needed to be elaborated upon and to be specific on the “demonstrate capabilities” and “Integrate SEI models.” The reviewer further inquired about the SEI models and capabilities.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer explained that the project is more fundamental and does not have as direct a connection to battery operation, use and management, but, it could provide very important fundamental insights and understanding that will improve performance and control in the longer timeframe.

Reviewer 2:

The reviewer described that the project goal is to address the causes and implications of thermal runaway in Li-ion batteries using a developed software package that can provide predictive mechanisms. The commenter affirmed that safety is a prime concern for large battery packs intended for transportation applications; thus, this project is well-aligned with DOE's goals.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer commented that \$1.5M per year is pretty high, but, the reviewer liked the collaboration with academia.

Reviewer 2:

The reviewer stated that little information regarding resources was presented. The presenter mentioned several times that they are the owner of the CANTERA open-source modeling package on which the project is based.

Coupling of Mechanical Behavior of Cell Components to Electrochemical-Thermal Models for Computer Aided Engineering of Batteries Under Abuse: Ahmad Pesaran (National Renewable Energy Laboratory) - es199

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

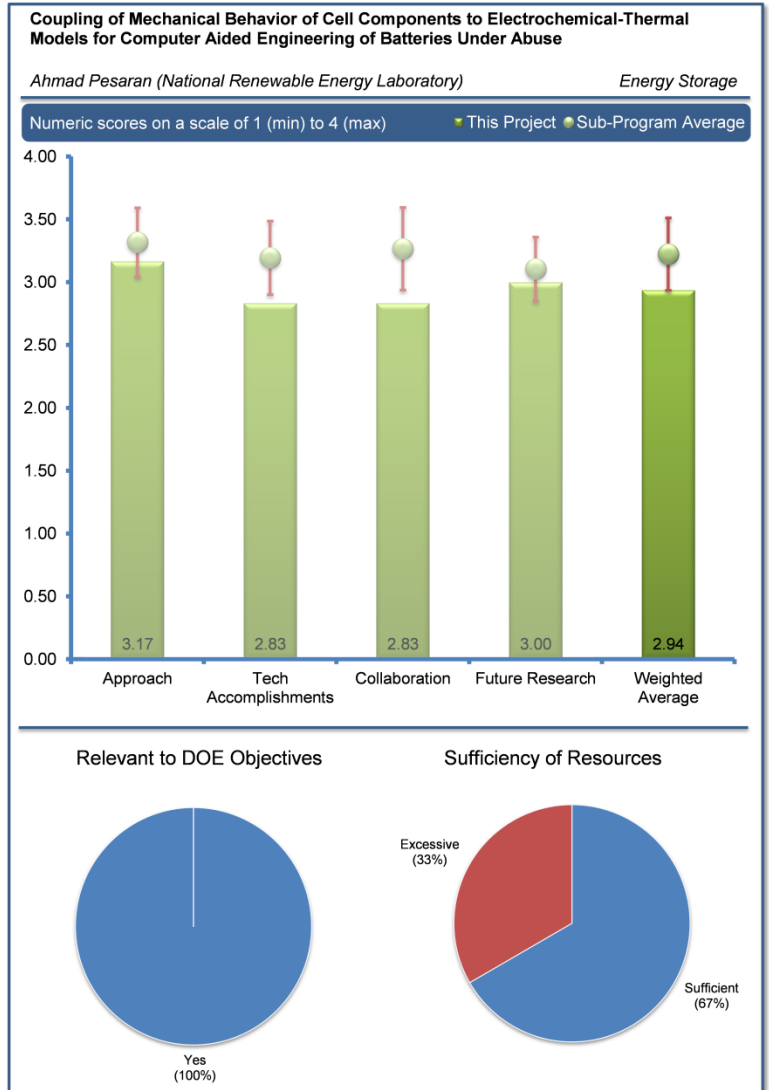
The reviewer indicated that the project was another in the set of highly needed technology progression into modeling of “Li-ion safety” in applications. The reviewer has a certain question as to the cell size and form factor frequented, particularly with MIT as a partner who has long term expertise in cylindrical characterization and crush modeling with uncertain transfer or validation toward large format and/or large module configurations.

Reviewer 2:

The reviewer stated that the approach was to couple the electrochemical-thermal (ECT) model with the mechanical deformation model to predict thermal response in a crush. However, since NREL’s Abuse Reaction Kinetics (ARK) model for thermal ramp is empirically based, the thermal ramp response will depend on cell design, for example high power versus high energy. The reviewer added that the project team’s bottom-up approach to build the cell thermal ramp rate from individual cell components heating rates was a good approach.

Reviewer 3:

The reviewer observed that the project will develop a model to couple the ECT behavior of a Li-ion cell with its structural behavior after rapid mechanical deformation using MIT's mechanical model. The reviewer stated that another model would also be developed to predict the thermal response of cells to thermal ramp. To do this, NREL's chemical kinetic abuse model would be transferred to the ANSYS CAEBAT-1 platform while including the actual internal geometry of cells. The reviewer commented that the modes would be compatible with CAEBAT-1 and the Open Architecture Software (OAS) developed by ORNL. The reviewer asked what the current limitations were of the MIT mechanical and NREL chemical kinetic abuse models. The reviewer also wanted to know if these limitations would hamper the extension of these models to these abuse tests. If so, the reviewer asked how this would be addressed.



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.**Reviewer 1:**

The reviewer indicated that the project team's data showed good correlation on the thermal ramp rate versus temperature ARC data with the simulation. The reviewer also said that it seemed reasonable to correlate resistivity with deformation during crush but it was not clear how the project team quantified deformation. The reviewer added that it was also not clear how the rate of resistivity change was used in the ECT model to predict thermal ramp during crush.

Reviewer 2:

The reviewer stated that a number of accomplishments were noted including the readiness to share the NREL Abuse Reaction Kinetics (ARK) model with ANSYS once the project team accepts the contract, the development of a user-friendly tool for parameter identification for the ARK model, a new enhanced anisotropic model of a cell jellyroll to aid in the coupling of the existing ECT model with the mechanical model, and compression testing of cells to obtain experimental validation data. The reviewer noted that one of the slides showed a tensile test on components of the electrode and separator assembly. Presumably there was no electrolyte present during the testing due to the solvent's volatility. The reviewer asked if the mechanical properties of the material would change significantly when soaked with electrolyte, for example, in a cell. The reviewer added that simulations were in progress to establish what parameters must be exchanged between the models. Some challenges and barriers were noted by the reviewer, including the difficulty of using the multi-layer puncture approach to capture damage zones created by different crush loads and orientations and the fact that model validation with experimental data may be complicated by the difficulty of matching.

Reviewer 3:

The reviewer could have rated this lower with not much progress. The reviewer was sorry to recognize the ANSYS issues as not necessarily trivial. The reviewer believed the NREL staff to be extremely competent and only hopes that the project team can get some forward synergy.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer noted that there was good collaboration with various teams and specific roles were described, but it was not clear if there is a good feedback loop between validation at NREL and the simulation from the team members.

Reviewer 2:

The reviewer indicated that the team was led by NREL's Energy Storage Team with collaborations with NREL's High Performance Computing Team, MIT and ANSYS. ANSYS has still not accepted the contract to work with NREL on this project. The reviewer added that this may delay the accomplishment of the project's future milestones, although the presentation indicated that this may not be the case. The difficulty here was unclear to this reviewer because ANSYS must have agreed to this partnership early in the proposal process and ANSYS was working with other partners for the CAEBAT projects. Also, the reviewer said that the direct discussions with OEMs about their experience with thermal runaway and crush testing and their desired output from a new model would perhaps be fruitful.

Reviewer 3:

The reviewer referenced prior comments.

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.**Reviewer 1:**

The reviewer listed the future plans: to transfer the ARK model to the CAEBAT-1 platform while maintaining OAS compatibility, validate thermal ramp abuse model with experimental data, and create and validate the couple mechanical deformation (crush)-ECT

model and transfer it to the CAEBAT-1 platform while maintaining OAS compatibility. The reviewer added that interactions with other groups which conduct thermal runaway and crush testing may be helpful for obtaining relevant experimental data in a timely manner.

Reviewer 2:

The reviewer agreed with the proposed future work though, that the project team should expand their abuse modeling to other abuses such as impact, shock or over discharge.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer said that the project addresses two battery abuse conditions (i.e., “crush” and “thermal ramp” runaway of cells). Given that safety is of paramount importance for transportation battery packs, the reviewer asserted that this project is highly relevant to DOE goals.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer noted that it was presumed that the team had the necessary resources to accomplish the proposed work.

Efficient Safety and Degradation Modeling of Automotive Li-ion Cells and Pack: Christian Shaffer (EC-Power) - es200

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

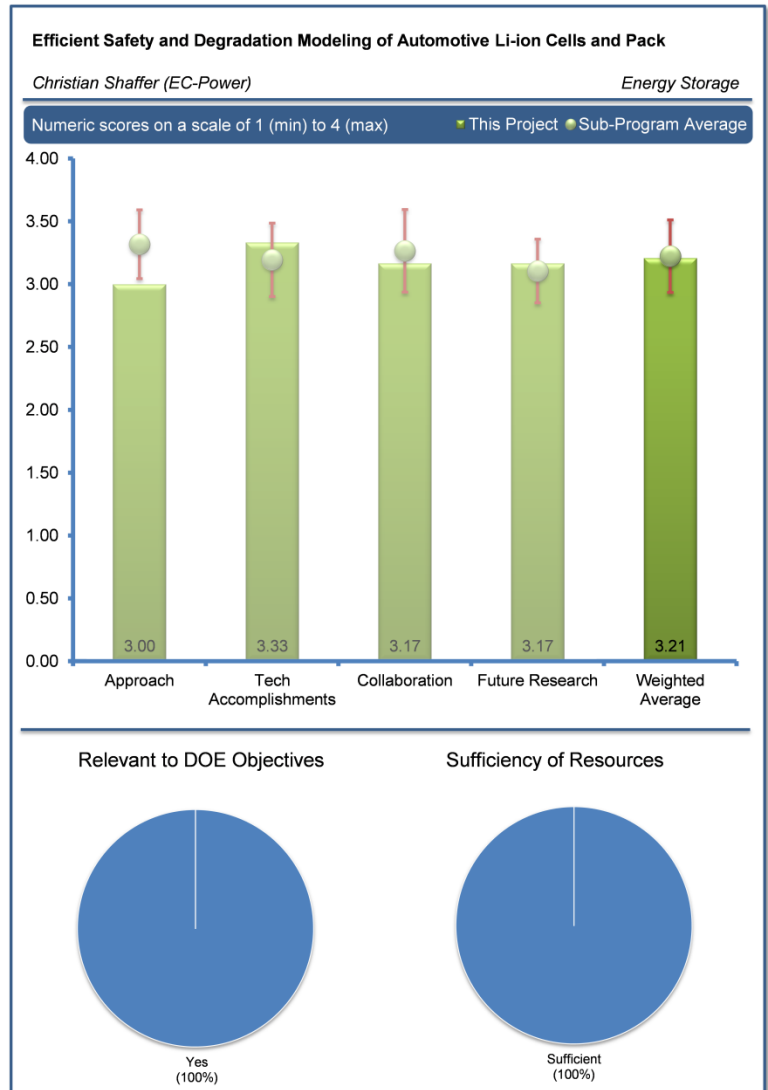
The reviewer stated that the major barriers and fundamental objectives identified were excellent. A robust pack-level safety and abuse model and mechanism-based, fundamental models for predicting degradation are essential; however, the reviewer warned that the focus on nail penetration (NP) as the model abuse initiation mechanism is of concern (by project definition you are using the NP not as an internal short representation but rather a true abuse). The reviewer explained that NP has become difficult to reproduce consistently from a physical hardware point of view, some have used the term “unreliable” but design sensitive to say the least. The reviewer indicated that this was largely due to advancement in production designs as opposed to 15 years ago, some may call “gaming” the design to pass a J2464 test but these design mechanisms are somewhat successful in safety improvements. So if the validation mechanism and model are to be of NP abuse, then the reviewer might challenge the project to broaden the nail material and size definition and speed to real world boundaries especially before module or pack level validation. The reviewer said cynically, a 35 mile per hour nail shot could be a bit scary.

Reviewer 2:

The reviewer mentioned that the model development would focus on cell safety, abuse and lifetime. The reviewer stated that little information was provided about what needed to be done to accomplish this. The reviewer asked what challenges were associated with this model development. The reviewer wanted to know if this would be readily integrated into the CAEBAT platform and the OAS developed by ORNL. The reviewer added that the project would expand the existing extensive materials database (developed by Pennsylvania State University's Electrochemical Engine Center (ECEC) previously) to include NCA. Large format cells would be prepared for experimental testing of safety, abuse and degradation.

Reviewer 3:

The reviewer indicated that the project team proposed to use the ECT model to predict life and combine ECT with pack level shorting model to predict Li-ion battery safety associated with shorting from nail penetration. Also, the reviewer noted that the ECT should be predictive since it is not empirical based and is based on parameters extracted from the extensive materials database. The reviewer added that it is not clear if the pack level shorting model will be applicable to other shorting induced incidents such as crush.



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.

Reviewer 1:

The reviewer commented that the NCA experimental property measurements are underway. Algorithms have been developed to efficiently simulate nail penetration of multi-cell packs. The reviewer asked if this includes the mechanical deformation of the cells from the nail penetration. Simulations have been run comparing the heating effects for one large graphite cell and the equivalent of six smaller cells assembled together (same voltage, same total capacity) to determine the effect of the number and arrangement of the cells within a battery pack. The reviewer added that the experimental nail penetration testing is being conducted to measure the detailed electrochemical and thermal responses (not just the variation in temperature). The reviewer stated that the initial model has been developed for enhanced life and abuse evaluation. Current work is focused on implementing the refined mechanism-based, temperature-dependent predictive models. The reviewer wanted to know what the principal limitations are of the current model. The reviewer also asked if it will be difficult to validate the model due to challenges in comparing experimental and simulated safety and abuse data and if so, how this will be addressed.

Reviewer 2:

The reviewer explained that the project team added NCA to the materials database. This will enhance the usefulness of the ECT model since NCA is a popular Li-ion cathode material. The reviewer said that the project team also developed a predictive life model that is mechanism-based and provided limited validation data. The reviewer added that it is not clear if the project team included electrolyte degradation in their life model. The reviewer reported that it will be very useful to extend the life model to include both storage calendar life and cycle life at various temperatures.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer indicated that there were excellent and well balanced partnerships on this project.

Reviewer 2:

The reviewer reported that there was good collaboration, but that it was not clear what the role of their other team member, Pennsylvania State University, was in this project. The reviewer added that it was also not clear how much of the ECT simulation could be performed in the OAS architecture.

Reviewer 3:

The reviewer indicated that the project was led by EC Power with a partnership with Pennsylvania State University. The reviewer added that no information was provided about the strength of this collaboration. The “Collaboration with Other Institutions” slide indicated that ORNL will provide the OAS. The reviewer stated that EC Power already worked with ORNL for the es120 project, development of cell and pack level models for CAEBAT-10, presumably this is a straightforward relationship. Interactions with other groups which conduct nail penetration testing may be helpful for obtaining relevant experimental data in a timely manner and for feedback about the simulation results.

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.

Reviewer 1:

The reviewer was pleased to see that the NCA cathode was considered in this project.

Reviewer 2:

The reviewer listed the proposed future research as complete the NCA characterization, Conduct the nail penetration testing and validation for single cells and multi-cell packs and to continue development and validation of the models for life and abuse testing (accelerated life and overcharge testing).

Reviewer 3:

The reviewer agreed with the project team's proposed research, but suggested to expand the abuse modeling to include other abuses such as over discharge and crush.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer stated that the goal of this project is to develop an efficient and robust pack-level safety and abuse model. The reviewer added that this will be a predictive, virtual tool with ECT coupling to assess, screen, predict cell, and pack design safety. Given that safety is of paramount importance for transportation battery packs, the reviewer said that this project is highly relevant to DOE goals.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer said that it is presumed that all necessary resources are available for the project since no information is provided regarding this.

Electrochemical Performance Testing: Ira Bloom (Argonne National Laboratory) - es201

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that the ANL's strong battery testing capabilities are derived from the laboratory's long experience in such testing and from being one of the key labs in setting up the protocols for battery testing.

Reviewer 2:

The reviewer indicated that the objective here is to provide DOE and the USABC with an independent assessment of contract deliverables of Li-ion cells from different developers for DOE/USABC, to benchmark external state-of-art battery technologies, and to project battery life. This reviewer added that standard USABC-developed testing methods are being applied to characterize cells, modules, and packs for determining performance at low temperatures (cold cranking), as well as cycle life and calendar life for projecting battery life. These results are being compared against the USABC goals to identify the gaps and shortfalls in the technology. Finally, continued the reviewer, these activities are being leveraged from similar activities in China to formulate consistent test protocols for EVs.

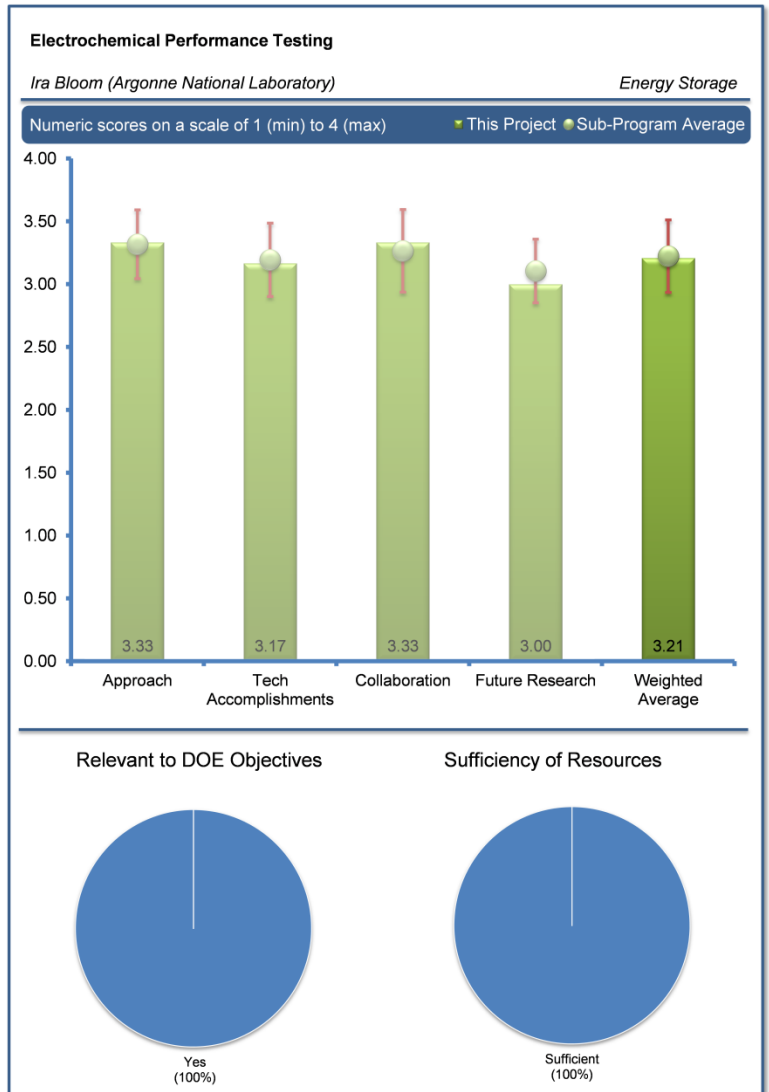
Reviewer 3:

The reviewer indicated that the ongoing work that ANL is doing in this area is very necessary and important. The reviewer added that the more recent integration of China Automotive Technology and Research Center (CATARC) collaboration is a great step in global standardization and comparisons. The reviewer fully supports this work and the very high level of ANL competence, though the reviewer was disappointed that this project was at the poster session without the PI present, leaving a technician to answer questions to only a very limited level and the reviewer came back several times.

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.

Reviewer 1:

The reviewer noted high quality, accurate measurements that characterize ANL's test data and the comparative data for China and United States tests used for this competency.



Reviewer 2:

Commensurate with a substantial funding being allocated for this project, this reviewer reported that several Li-ion technologies from different suppliers are being evaluated both at ANL and INL. It would be beneficial to the reviewer and to the community if the test results were briefly described. The reviewer indicated that test articles are mostly cells representing different technologies, with advanced anodes and cathodes, being developed for DOE. Although this reviewer acknowledged that it is important to perform independent verification of these “advanced technologies,” the selection of the technologies for this expensive and elaborate testing is not well thought out. The reviewer opined that this project should be more selective to pick technologies of merit of any viability for integration into EVs, rather than just being a verification center for the advanced technologies. Substantial effort, as observed by this reviewer, is being expended on comparing the U.S. and Chinese test protocols because the differences do not seem to be significant and this project can stick to one USABC protocol to test the hardware either from the United States or from China. This reviewer further added that there is not much anyone can make out of the effects of fast charge, unless the chemistry (1 and 2) is spelled out. The reviewer strongly expressed uncertainty as to why this information could not be revealed if these are commercial cells.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer observed useful collaborations amongst DOE laboratories and with international partners.

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.

Reviewer 1:

The reviewer stated that the project team was well-known for extensive collaboration with various national and international laboratories and developers.

Reviewer 2:

This reviewer commented that the proposed future research involves continued support of the DOE and USABC battery development efforts by performing independent assessment of contract deliverables using standardized test protocols, and providing results and feedback to the contractors. Further, the reviewer explained that plans include completion of the comparison of the USABC and China test protocols and to complete the studies on the effects of fast charge. As mentioned previously, the reviewer suggested that the objective of this project should be much broader (i.e., to make a thorough assessment of the current and upcoming technologies and to identify “technology gaps and shortfalls”) to guide DOE and USABC towards successful development of lithium batteries for EV applications.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer commented that ANL played a key role like INL for battery testing and validation. The reviewer added that ANL set the standards for battery testing.

Reviewer 2:

The reviewer explained the importance of performing a detailed independent assessment of available Li-ion battery technologies to demonstrate the technology advancements for DOE, advise USABC on the applicability of the batteries, and enable a timely infusion of Li-ion batteries into electric vehicles. This reviewer further noted that various performance metrics need to be established based on the anticipated use, and verified both at cell and module level (i.e., power and energy densities, cycle life [1,000-300,000 depending on application], calendar life [15 years], and low-temperature performance). The reviewer asserted that this project is duly addressing this need with a concerted assessment both at ANL and INL.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

This reviewer noted adequate resources for the scope of the project.

INL Electrochemical Performance Testing: Jon Christophersen (Idaho National Laboratory) - es202

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that INL represented the benchmark for battery testing and validation.

Reviewer 2:

The reviewer explained that the project objective is to provide DOE and the USABC with an independent assessment of contract deliverables of Li-ion cells from different developers for DOE/USABC, benchmark external state-of-art battery technologies, and project battery life. Other objectives reported by the reviewer are to develop advanced state-of-health assessment capabilities for Li-ion cells, to generate internationally accepted manuals for performance assessment of energy storage systems, as well as test and analysis protocols based on program targets and objectives. The reviewer summarized that the approach involves the following: testing both battery and ultracapacitor technologies in cells, modules, and full-size vehicle systems; developing advanced modeling and diagnostic tools; and exploring the basic issues of battery aging, performance, and prognostics in support of battery life estimation and state-of-health assessment capabilities using novel sensor technology. This reviewer asserted that the objectives and approach are consistent with the goals of ABR.

Reviewer 3:

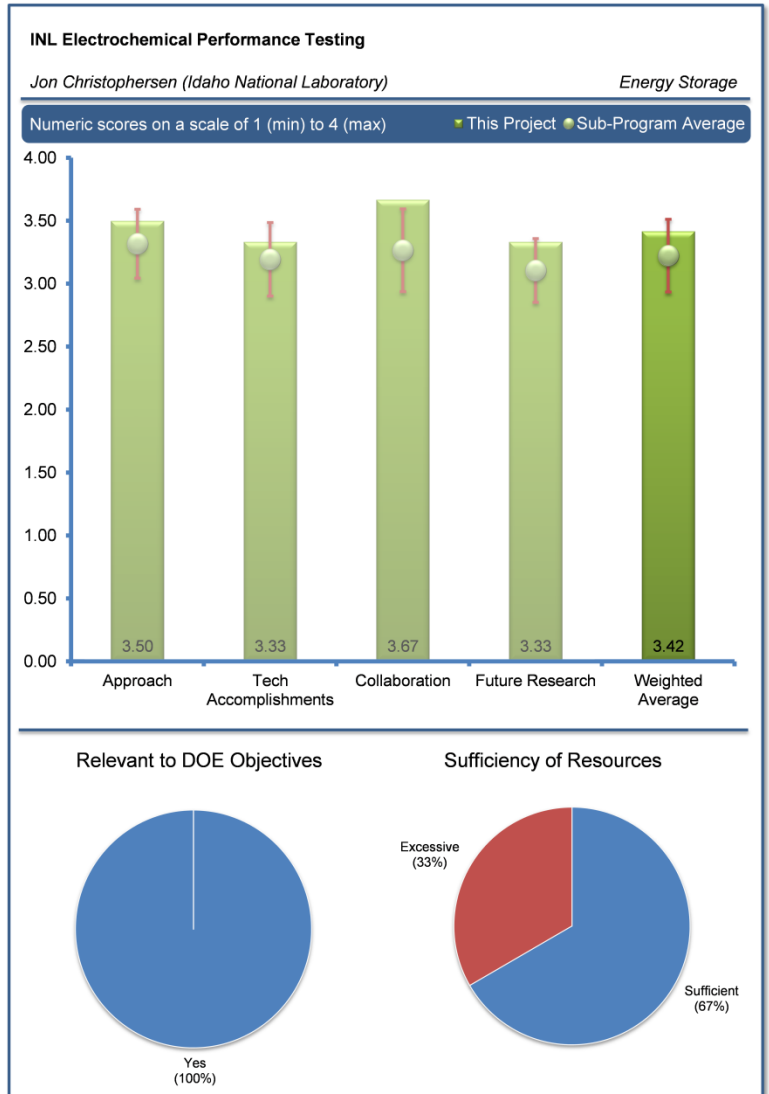
The reviewer indicated that quality testing, validation, and analysis were critical to the successful integration and adaptation of xEV into transportation. The reviewer added that ANLs support of USABC was significant to meet the greater objective.

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.

Reviewer 1:

The reviewer commented that the results from INL tests were of high quality and this feedback received by the developers were of tremendous value in the case of their battery development.

The reviewer explained that extensive facilities were set up with multiple test stations for performance testing of cells and modules with environmental chambers and packs, and also for vibration testing of batteries. Several test articles (i.e., cells and packs from the deliverables) were tested in support of the DOE/USABC contracts, but the reviewer criticized that information on these cells/batteries



was sadly missing in the presentation. The commenter proposed that it would have been useful to make a proper assessment of this effort and the technology development overall, if these findings (i.e., the test results from these cells and batteries) were published, especially if they are supported by DOE funds. The reviewer expressed that another noteworthy, though not entirely novel, accomplishment from this project was the development of a prototype 50-V impedance measurement box for assessing the changes in the EIS of cells in different architectures (i.e., series versus parallel) and as a function of calendar life at different temperatures. In closing, this reviewer noted that several manuals were published on the battery testing methodologies and performance simulations.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the collaborative effort of the national laboratories is critical to xEV success and, again, through USABC; it was a complete set.

Reviewer 2:

The reviewer reported that there was significant collaboration with many other national and other laboratories.

Reviewer 3:

The reviewer observed useful collaborations with other DOE laboratories (i.e., ANL, SNL, and NREL), USABC partners, and university partners were present.

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.

Reviewer 1:

The reviewer described that the proposed future research is to continue to support the DOE and USABC battery development efforts by performing performance tests on the existing and upcoming contract deliverables, and by providing the results and feedback to the contractors. The commenter also noted that the future plans include generating manuals for PHEVs, EVs, and micro-hybrid (48 VDC) batteries that incorporate the vibration system for batteries and to expand the battery-modeling capability. The reviewer highlighted that, together with the ANL's efforts (Bloom, et. al), this project is crucial in verifying of the performance of the current and emerging Li-ion battery technologies, for their successful infusion in electric vehicles.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer observed that the INL plays an important role in benchmarking and testing cells and batteries from around the globe. In addition, the reviewer said that INL's contribution towards developing test manuals for various power sources cannot be overemphasized.

Reviewer 2:

The reviewer explained that it is important to verify the various performance characteristics of different Li-ion battery technologies, i.e., the technologies being developed by DOE/USABC as well as the technologies developed elsewhere for their applicability in electric vehicles. The reviewer proposed that various performance metrics need to be established, based on the anticipated use and verified both at cell and module level, i.e., power and energy densities, cycle life (1,000-300,000 depending on application), calendar life (15 years), and low-temperature performance. The commenter confirmed that this project is fulfilling this need with a concerted effort both at INL and ANL.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer commented that the resources seem to be slightly excessive, although the scope of the project is fairly broad.

Battery Safety Testing: Christopher Orendorff (Sandia National Laboratories) - es203

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer indicated that the SNL was uniquely qualified for and focused on carrying out abuse-testing with the highest degree of planning and thoroughness.

Reviewer 2:

The reviewer reported that this project was one of the national laboratory's key collaborative efforts to support USABC and the technology growth, through understanding abuse conditions and characterization.

Reviewer 3:

The reviewer explained that the project objective is to provide DOE and the USABC with a detailed assessment of the abuse tolerance of the contract deliverables of Li-ion cells from different developers for DOE/USABC per USABC testing procedures to evaluate single point failure propagation in multi-cell batteries, to understand the effect of aging on abuse tolerance, and to verify the mechanical model predictions on the crash-tolerance of EVs. The reviewer also stated that accelerated rate calorimetry work is being performed at the cell level to characterize different chemistries. The reviewer also reported that thermal and mechanical failures are being assessed in modules and battery packs with the elaborate and exclusive facilities set up at SNL for DOE and USABC. The reviewer described that these activities are well-integrated with other developmental activities and are consistent with the overall program objective to address the safety, which is one of the technical barriers. Unfortunately, the reviewer said that the results from these studies were being treated as confidential with the test articles developed for DOE (with DOE support), or even with commercial test articles.

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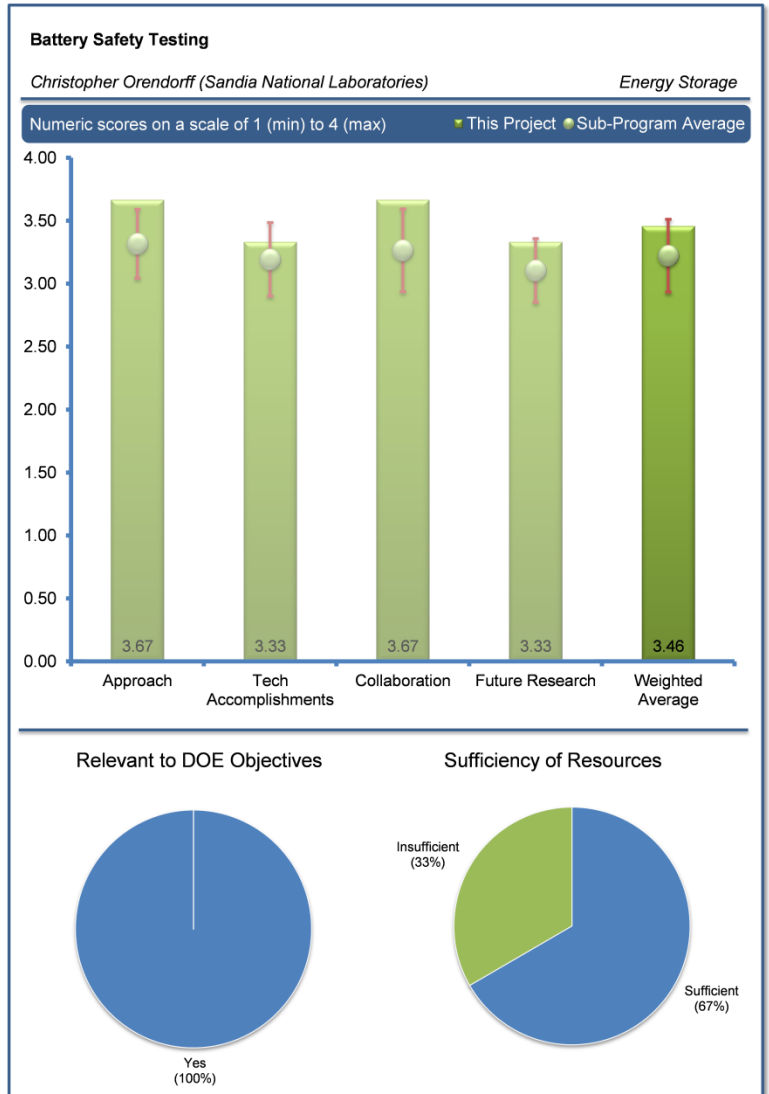
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer said that a significant number of cells, modules, and packs had been characterized with respect to their abuse-tolerance. The reviewer added that these results were extremely valuable feedback to the developers.

Reviewer 2:

The reviewer affirmed that good progress was being made in evaluating various cells and battery packs that were supplied as deliverables from the USABC program, as may be expected from the healthy funding allocated for this project. The reviewer explained that the test articles are mostly cells and multi-cell packs that represent different technologies, including some with advanced anodes and cathodes,



which are being developed for DOE. In addition, the reviewer reported that the effects of aging in single cells and cell failure propagation paths in parallel series configuration were studied. Finally, the reviewer indicated that the test procedures have been developed for mechanical abuse and crash simulation tests were performed in support of mechanical models. One difficulty the reviewer had with the safety testing in general is that the safety events in field use are always different from the simulated abuse tests and the response is often difficult to predict.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer commented that there was extensive collaboration with all relevant developers from inland and overseas.

Reviewer 2:

The reviewer acknowledged that there are useful collaborations amongst DOE laboratories and with USABC partners.

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.

Reviewer 1:

The reviewer noted that one area that SNL should improve its expertise was in the analysis of gases during and after abuse-testing. This was especially true for quantitative analysis of large format cells.

Reviewer 2:

The reviewer summarized that the proposed future research is to continue to support the DOE and USABC battery development efforts by performing abuse testing of contract deliverables, and providing the results and feedback to the contractors. Further, the reviewer noted that the future plans include propagation testing of batteries with increasing levels of designed passive and active thermal management to demonstrate the effectiveness of engineering controls to mitigate propagation and to determine the chemistry modifications and effects of aging on the thermal propagation. The reviewer also explained that the selected batteries will be subjected to dynamic mechanical testing for verifying the model and to demonstrate battery crashworthiness of EVs (for USCAR). The reviewer agreed that these studies will address the safety or abuse tolerance of Li-ion batteries, for a successful infusion of lithium batteries in electric vehicles.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer observed that the SNL plays a very important role in the development of abuse-tolerant battery packs.

Reviewer 2:

The reviewer highlighted that, in addition to high specific energy and long life, adequate safety is an important requirement for Li-ion cells in EV applications. The reviewer explained that as newer chemistries are being developed, their safety characteristics are even less understood so warrant a systematic assessment of the emerging technologies both at the cell level and battery level. The reviewer specified that the abuse condition may be induced electrically, thermally, and/or mechanically to simulate failures that are occurring in the field. The project evaluator agreed that this project is duly addressing this need with a focused safety assessment under different abuse conditions of various technologies being developed by DOE/USABC.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer explained that additional funding could greatly accelerate needed propagation testing and development efforts.

Reviewer 2:

The reviewer simply stated that the resources are adequate for the scope of the project.

Battery Thermal Characterization: Matthew Keyser (National Renewable Energy Laboratory) - es204

Reviewer Sample Size

A total of two reviewers evaluated this project.

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.

Reviewer 1:

The reviewer remarked that NREL was the go-to laboratory for and the authority on thermal characterization of cells, modules and packs. The reviewer stated that NREL’s approaches were innovative and well-organized.

Reviewer 2:

The reviewer indicated that the PI, an enthusiastic sort by the way, has taken the correct approach when looking at or observing useable ranges of the devices under evaluation. The reviewer hoped that did not curtail a greater objective to broaden the useable range for increased performance 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.

Reviewer 1:

The reviewer stated that NREL's test data was very comprehensive, has a high level of accuracy and reproducibility, thus furnishing valuable information to developers.

Question 3: Collaboration and coordination with other institutions.

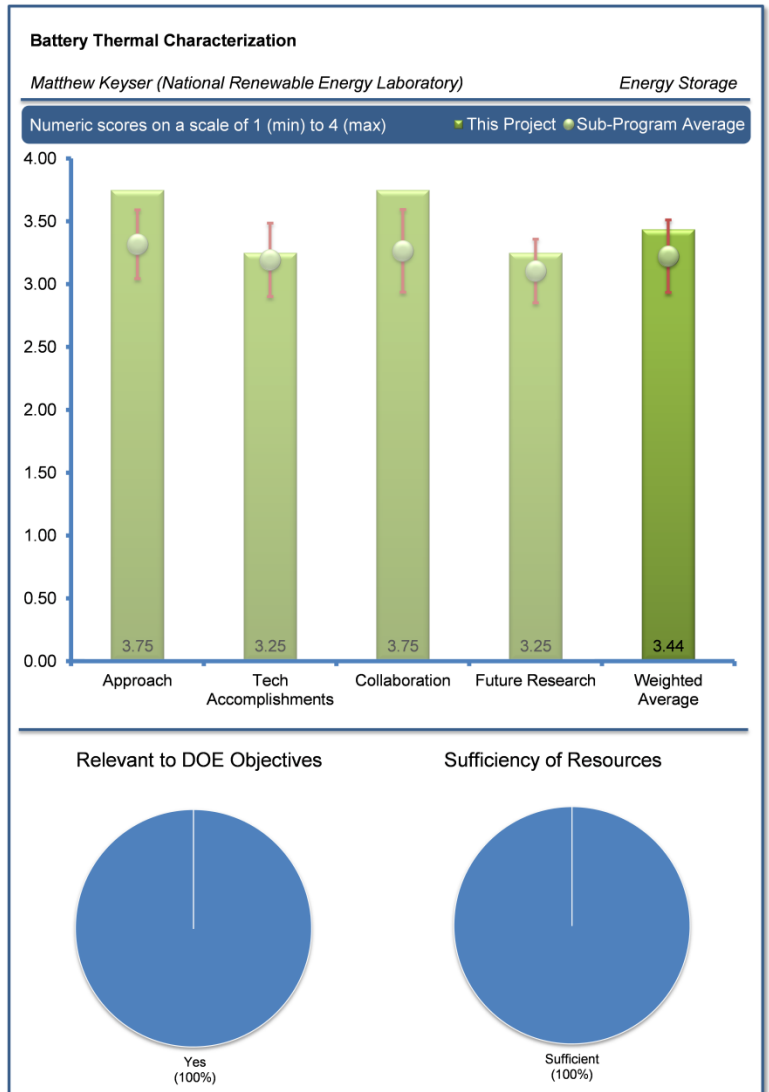
Reviewer 1:

The reviewer indicated that there was extensive collaboration with various developers and laboratories.

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.

Reviewer 1:

The reviewer said that again, NREL has developed time-tested methodologies for their work.



Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer stated that NREL served a critical role in the overall characterization and understanding of energy storage technologies.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

No comments were received in response to this question.

Advanced Battery Recycling: Steven Sloop (OnTo Technology) - es205

Reviewer Sample Size

A total of two reviewers evaluated this project.

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.

Reviewer 1:

The reviewer indicated that the approach was innovative and clearly focused on achieving the specific objectives set forth by the proposal. The reviewer added that it would have been beneficial to have included more of a cost analysis task in the research, although this may be suitable for a follow-on activity.

Reviewer 2:

The reviewer reported that since not much was known about the process deployed to rejuvenate the materials, one could only make general comments that the approach seemed to be appropriate since it was achieving the target material through the recovery process.

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.

Reviewer 1:

The reviewer stated that the data seemed quite exciting, showing excellent recovery of the cathode capacity. Because of interest in the recovered capacities, the reviewer encouraged the authors to display the data in absolute terms without normalizing. The reviewer added that more comprehensive rate and capacity data should be part of the data collection package.

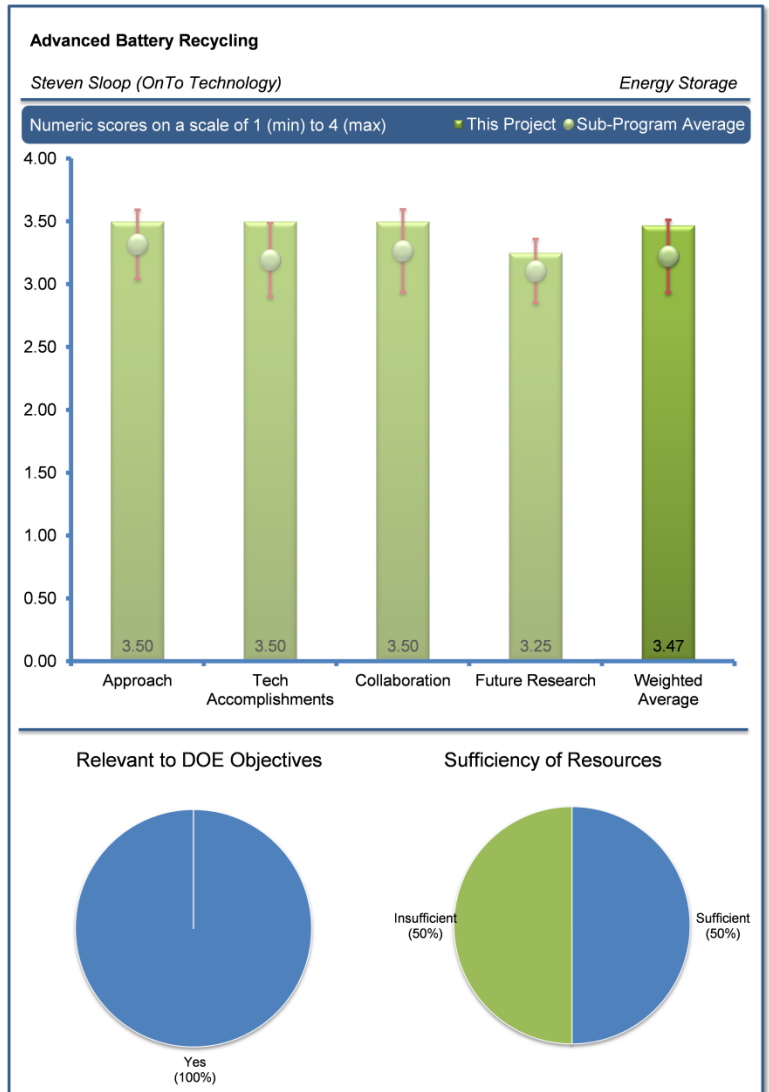
Reviewer 2:

The reviewer remarked that the accomplishments were impressive. The reviewer added that the majority of the program focused on process development, and that the data shown was encouraging. Also, the reviewer said that it would be helpful if the investigator could comment on the formulations and types of cathodes used in the study. The reviewer understood that most were NMC-type, but there were different NMCs, and many EV cells were currently blended with Lithium Manganese Oxide (LMO) spinel. The reviewer explained that the effect of such blends on this process and the optimum formulation of the resultant cathode product would be beneficial to the review.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer indicated that the appropriate partners were involved as collaborators.



Reviewer 2:

The reviewer reported that the collaboration was very clear, which was essential for program success.

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.

Reviewer 1:

The reviewer stated that high temperature storage and cycling should be part of future studies as well as transition metal dissolution studies. The reviewer added that it would be really interesting to see whether the material survived the second round of rejuvenation.

Reviewer 2:

The reviewer suggested that the future work should focus on stabilization and optimization of process, for control of material, repeatability. The reviewer added that the investigator should also provide a preliminary techno-economic analysis for the final process. This reviewer also wanted to know how effective such methods might be if they were applied to advanced anodes.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer pointed out that the importance of this program could hardly be overemphasized. The reviewer added that this was a very important part of the overall development, production, use, and recycle strategies that needs to be developed for efficient, cost-effective development and use of vehicular batteries.

Reviewer 2:

The reviewer acknowledged that an opportunity exists to develop a recycling approach analogous to lead-acid. Also, the reviewer stated that this addressed at least the single most costly material in a Li-ion cell.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer recommended a higher level of funding for this important project.

Reviewer 2:

The reviewer pointed out that there were no issues and that this was a well-balanced project.

Real-time Metrology for Li-ion Battery R&D and Manufacturing: Jong Yoo (Applied Spectra) - es206

Reviewer Sample Size

A total of two reviewers evaluated this project.

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.

Reviewer 1:

The viewer indicated that the approach appeared interesting provided it could meet manufacturing and cost targets: acquisition and response time, data reliability, accuracy etc. The reviewer said that knowledge about the spatial distribution of various cell and electrode components is very useful for designing efficient electrodes.

Reviewer 2:

The reviewer reported that the investigator has applied an effective approach to the implementation of Laser-induced breakdown spectroscopy (LIBS) to li-ion and related battery technology. The reviewer added that the investigator is also well on the way to achieving the goal of a user friendly device.

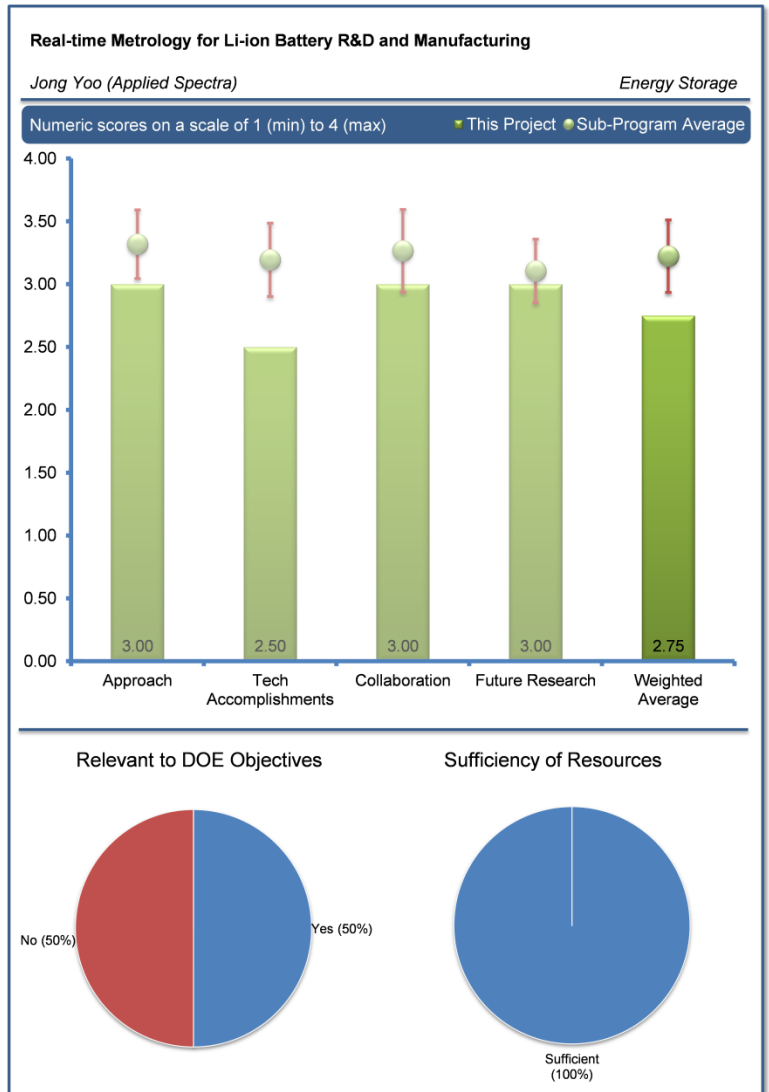
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer remarked that the data for carbon or Polyvinylidene difluoride (PVDF) in the electrodes provides a good opportunity to analyze the quality of electrodes. The reviewer stated that it would have been better if the authors would have provided any correlation between the various spectra and the composition of the electrodes to see if one could use this technique to monitor the quality of the electrodes. As the reviewer mentioned earlier, it is not clear that this technique can be deployed as an in-line QC tool, because it needs to provide rapid analysis so that there could be some feedback to tweak the composition if needed. The reviewer added that it could still be a powerful off-line technique provided its response time, accuracy, and cost are superior to competing techniques.

Reviewer 2:

The reviewer explained that this is an analytical tool and it operates through a destructive analysis process. The reviewer added that the tool has the ability to provide insight into compositional and structural variation. The reviewer indicated that it is not clear from the investigation how this tool and the analytical data it generates complement other test methods. Also, the reviewer suggested that the investigator should focus on demonstrating a case study where the LIBS technique is used to support investigations with other analytical methods.



Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer stated that LBNL can provide excellent feedback on various technical issues.

Reviewer 2:

The reviewer reported that the breakdown of work responsibilities was not clear.

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.**Reviewer 1:**

The reviewer noted that a 3D analysis of begin-of-life and end-of-life electrodes should be a part of the project.

Reviewer 2:

The reviewer encourages the investigator to also demonstrate the LIBS technique complementary with other analytical techniques.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer said that the project team had a good understanding of the electrode composition and structure as a requirement for building efficient batteries.

Reviewer 2:

The reviewer remarked that it is not clear how significant an improvement to a manufacturing process would result from the inclusion of this analysis tool.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that the project is nearing completion, and that no issues were seen.

Manufacturability Study and Scale-Up: Claus Daniel (Oak Ridge National Laboratory) - es207

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer indicated that the project was keenly focused on benchmarking against commercial materials and processes and developing a domestic supply chain network. Also, the reviewer pointed out that great effort was put into bringing in external staff to address the team's internal limitations.

Reviewer 2:

The reviewer observed that the technical approach appears sound in terms of validating advanced manufacturing processes used in Li-ion technology. The reviewer added that this group is also a receiving entity for new materials developed in other domains of the DOE materials which allows the overall evaluation of materials in a complete system. While this is clearly an important aspect of moving the overall technology forward, and a well done aspect of this goal, a separate stated goal of the program is that of ultimate cost reduction. The reviewer is less convinced that this program will address that particular goal, but the reviewer saw the value of the program despite this concern.

Reviewer 3:

The reviewer indicated that the right equipment is in place and the general areas are good. It is a good thing for ABR partners with no cell capability if any. The reviewer would prefer to see them work on more advanced materials, but the reviewer stated that the project team is still using well known materials to be sure they are getting good product manufactured.

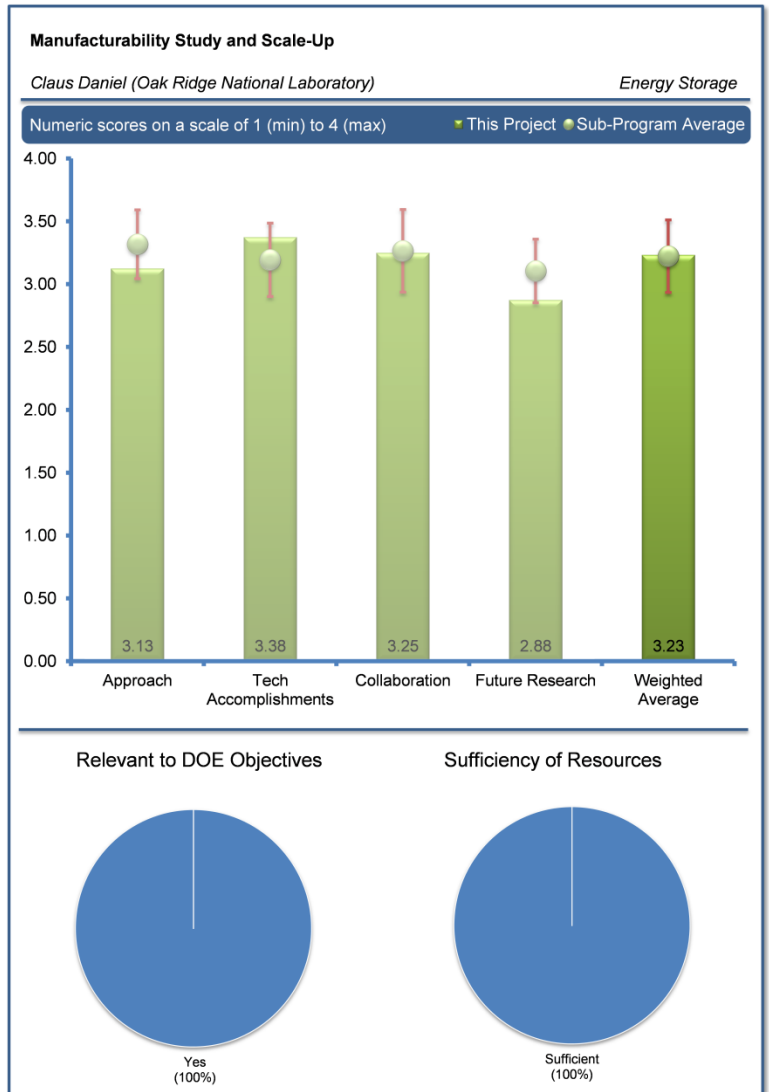
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer stated that the group is providing the component quantities that were set at the milestone level.

Reviewer 2:

The reviewer claimed that the project team has clearly learned a lot about making cells. A lot of equipment was installed, they made a number of cells and thousands of feet of electrodes. The reviewer pointed out that large cells are still lacking somewhat in durability. The reviewer said that work on improving yield could bear fruit.



Reviewer 3:

The reviewer indicated that the project team has met all project milestones to date, and are working on their fourth quarter FY 2014 milestone. The reviewer commented that the project team should develop a more quantitative metric of technology development. The reviewer added that qualitatively it looked like the technology commercialization strategy was progressing.

Reviewer 4:

The reviewer said that the project team setup manufacturing facilities for electrodes (both anodes and cathodes) and produce large areas of coated electrodes and test them in pouch cells.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer stated that the project team had aligned scaled up work which was being done at ANL. The reviewer added that the project team has targeted other facilities for their analytical capabilities and that the project team is using commercial equipment to get results that can be translated out to commercial partners.

Reviewer 2:

The reviewer commented that the collaboration is occurring with domestic cell producers, materials suppliers, and etc. The reviewer said that a comment from the partners on the value of the work might be appropriate at future meetings.

Reviewer 3:

The reviewer stated that the facility itself involved a number of industrial partners.

Reviewer 4:

The reviewer indicated that the partners seemed to be consultants, customers or suppliers. The reviewer noted that the project team needed to engage partners as partners who work together with ORNL, and maybe each other, to really make gains that matter to the economy and the people. The reviewer added that in questions, the presenter said that the project team had people in to work, but it still sounded like that was the exception. According to the reviewer, to succeed in getting a supply chain built, this work needed to be significantly more interactive and have partners working on site and learning all the time.

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.**Reviewer 1:**

The reviewer stated that, given the project successes to date, it appeared that continuing along and doing more of the same with this kind of user facility would lead to project success. The reviewer said that while the project was scheduled to go until FY 2016 it was unclear what the milestones would be. The reviewer added that future work could be better defined and planned, currently quite nebulous.

Reviewer 2:

This reviewer indicated that the project team had logical and reasonable future goals.

Reviewer 3:

The reviewer observed that the plans were not very detailed. The focuses noted were good ideas but there was not an integrated plan. The reviewer said that this was a great facility, the project team should set a virtuous goal and work to accomplish it, and in doing so, include a set of meaningful U.S. partners as active participants in the work.

Reviewer 4:

The reviewer recommended that the facility work with several academic institutions for new materials and processes. The reviewer also said that the pilot scale facilities established here seemed to follow the well-established processes and materials. So, it was important to introduce new processes developed at some of the academic institutions for introducing new materials in to Li-ion battery production.

Otherwise, the value of these facilities may be limited in the long run when industrial partners build their own facilities in the United States.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer stated that with the correct objectives, this was a valuable capability in the overall goal of moving the Li-ion technology forward.

Reviewer 2:

The reviewer said that manufacturing research was very relevant to cutting down the battery costs.

Reviewer 3:

The reviewer pointed out that advanced batteries consisted of a large number of materials. Being able to source these materials domestically will be the key to growing America's manufacturing capabilities. The reviewer added that addressing these scale-up issues will ultimately allow batteries to displace petroleum.

Reviewer 4:

The reviewer remarked that the project helped the DOE and researchers under contract to make better estimates of the true cost. The reviewer added that if it was clear this was moving advanced materials to commerce it would be incredibly relevant, but it was not clear how much of this would be used by the battery making partners.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer encouraged the continued funding of this program, especially if it continued to bring in matching external funds.

New High-Energy Electrochemical Couple for Automotive Applications: Khalil Amine (Argonne National Laboratory) - es208

Reviewer Sample Size

A total of seven reviewers evaluated this project.

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.

Reviewer 1:

The reviewer indicated that the project was being carried out by a strong technical team led by a well-established scientist, Dr. Khalil Amine with expertise in all aspects of battery research such as electrode materials, binders, and electrolytes, as well as strong characterization capabilities at ANL and BNL. The reviewer added that the project goals were clearly defined and milestones were on schedule.

Reviewer 2:

The reviewer pointed out that the project team had a clear strategy and approach to address the problems. The reviewer added that existing knowledge was good basis to solve challenges.

Reviewer 3:

The reviewer said that in this project, the PIs were developing full concentration gradient (FCG) NMC cathode and Sn-Si composite anode for high energy density battery greater than 250 W/Kg.

Reviewer 4:

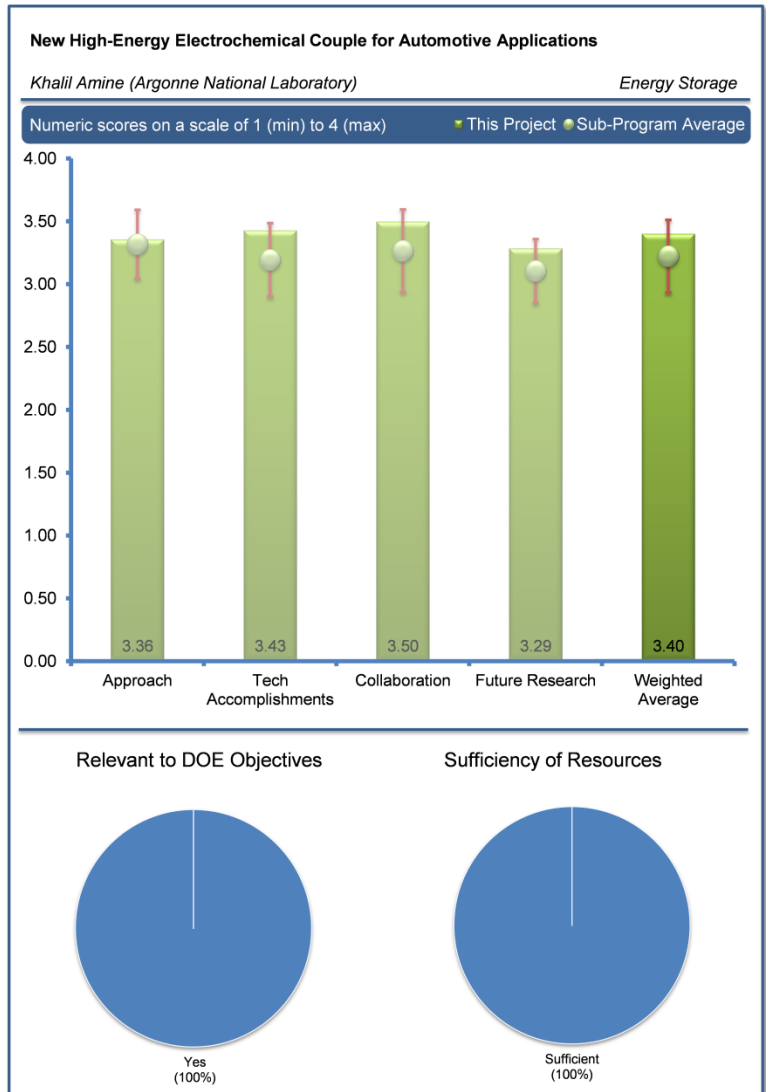
The reviewer noted that the preliminary work by the PI and Professor Sun has shown good properties of the FCG NMC material and it is appropriate to evaluate it in full cells to test actual performance in various possible applications. The reviewer added that the choice of anode has led to a large irreversible capacity so it may be useful to extend the work to graphite cells and pure silicon, or modified silicon, in addition to the SiO combination with the Sony tin alloy. This may allow separation of anode and cathode effects since it is well known that these system types can have strong interactions between anode and cathode.

Reviewer 5:

The reviewer reported that the gradient concentration materials were unique and a counterpart to the approach of Mn-rich shells. The reviewer added that the preparation of the materials was based on a batch process obviously, although a continuous product was possible in theory; however, a scale up appeared to be correspondingly challenging.

Reviewer 6:

The reviewer commented that the specific challenges associated with each of the new components and system as a whole could be defined a little better. The reviewer added that as always, cost projections would be useful to help guide the practicality of the system.



Reviewer 7:

The reviewer commented that it was not completely clear how this FCG material is synthesized. The commenter noted that the authors mentioned that the powders can be synthesized by using carbonates or NaOH in a continuously stirred tank reactor (CSTR) process; however, if the process starts with water only (at the beginning of the process), some of the initial material will not be produced at steady state and will have to be discarded. Furthermore, the reviewer described that the process will have to run for a short period of time (or until the metal solution reach the maximum Mn concentration, a point where the process will have to be stopped). The reviewer asked how much material is out of spec and being lost. The commenter suggested that the synthesis can also proceed through a CSTR-batch process, where nothing is discarded and the process is stopped after the metal feeding solutions reach the maximum in Mn concentration; in this case none of the material is lost. The reviewer requested that the authors should explain further how practical is their synthetic method.

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.**Reviewer 1:**

The reviewer commented that the results had been presented in a consistent, meaningful and complete way. The reviewer added that taking into account the elapsed time, the amount of results was astonishing.

Reviewer 2:

The reviewer claimed that it was early in the program; however, good progress was observed in terms of establishing baseline performance and the early stage synthesis of key components.

Reviewer 3:

The reviewer stated that the project had just started and showed good preliminary results.

Reviewer 4:

The reviewer said that the team had carried out a large amount of work in making and evaluating anode and cathode materials as planned. The team has identified “Remaining Challenges and Barriers.” The reviewer added that after the first year of the project, the team may reevaluate its future plans to focus on overcoming challenges and barriers. Specifically, it is unclear why conducting polymer binder should be a focus because the $\text{Sn}_y\text{Co}_{1-x}\text{Fe}_x\text{C}$ alloy should be electronically conducting. Also, the reviewer stated that the team should also put more effort on characterizing the composition and structure of the ball-milled $\text{SiO-Sn}_y\text{Co}_{1-x}\text{Fe}_x\text{C}$. The claim of “possible alloying between Si and Sn” is intriguing because equilibrium phases do not exist in the Si-Sn binary system. The reviewer asked if the ball-milled material is a single phase alloy or a multiple phase composite and if it is amorphous. The reviewer wanted to know where the oxygen is after ball milling. Also, the reviewer asked if the oxygen in the “alloy” was the cause of the irreversible loss. If so, the team needed to consider alternative anodes.

Reviewer 5:

The reviewer observed that the work to date has set the stage for the construction of full cells. The reviewer would like to see the full cell evaluations carried out in sealed pouch cells or cylindrical cells rather than the coin cells utilized in the early work, particularly for cycle life tests. The reviewer added that the use of SiO guarantees the high irreversible capacity of the anode unless only very small proportion is used in comparison to the Sony material. The reviewer hopes that a more satisfactory anode component can be devised to minimize the irreversible anode capacity. This may involve a more conventional binder such as carboxymethyl cellulose (CMC) at least as a baseline material.

Reviewer 6:

The reviewer observed good accomplishments with plenty of data and positive results for a proof of concept; however, rate capability was still in question although it was still in an early stage.

Reviewer 7:

The reviewer indicated that the accomplishments with cathode materials seemed reasonable. The reviewer said that it was not clear about the anode and the processing method used. Also, the reviewer stated that both the performance of FCG NMC cathode materials and the processing technique needed to be established.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer noted that there was a good collaboration network with a wide range of expertise.

Reviewer 2:

The reviewer indicated that the collaboration was well balanced and effective, not too many partners. The reviewer added that there was a consortium with the necessary skills on board. A partner for industrialization or end-user would have been great. The reviewer noted that the approach for anode and electrolyte were quite similar to the 3M and Envia project. The reviewer said that a comparison of results across the board of those projects would be interesting.

Reviewer 3:

The reviewer said that the team was quite competent and had access to all of the resources necessary to run a complex materials and cell development program.

Reviewer 4:

The reviewer agreed that the collaboration seems to be good.

Reviewer 5:

The reviewer stated that collaboration was very appropriate to the work. Dr. Yang and Professor Sun were key figures in achieving the cathode materials and Dr. Liu and others would contribute to the anode work.

Reviewer 6:

The reviewer stated that collaboration with others was not well defined other than those involved in the project.

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.**Reviewer 1:**

The reviewer observed that the proposed next steps were focused on main challenges and suitable to overcome the key barriers. The reviewer added that the efforts in investigation of thermal stability and safety are of major importance. Also, the reviewer remarked that cost prognosis relative to state-of-the-art would be beneficial.

Reviewer 2:

The reviewer indicated that it was a good idea to try the 622 as a baseline cathode powder. The reviewer added that the authors would have the opportunity to better understand this important high capacity powder, in addition to the gradient materials.

Reviewer 3:

The reviewer stated that the use of a pouch cell approach would be valuable to truly assess the system. The reviewer added that the suggestions above concerning the anode were the key to obtaining high energy density. The reviewer said that the work proposed by the PI was important to continue as well.

Reviewer 4:

The reviewer agreed that it was a good idea to try the 622 as a baseline cathode powder. The commenter explained that the authors will have the opportunity to better understand this important high capacity powder, in addition to gradient materials. The reviewer suggested

that it could be of interest to show data on the rate of discharge, in particular of the cathode powders. The reviewer concluded by asserting that third-party verification of future results should be in place.

Reviewer 5:

The reviewer stated that the project team may consider the questions the reviewer raised in Part 2.

Reviewer 6:

The reviewer would have liked to see some data beyond the proof of concept and characterization data. For example, cycle life data and rate capability data can provide more convincing path for further optimization and development. The reviewer then asked if there was any cost analysis and projection plan.

Reviewer 7:

The reviewer said that the scale-up of proposed anode materials was not clear. In fact, it was not clear on why the PIs chose this type of anode material. Both the composition and the processing method seemed complicated. The reviewer indicated that the performance of FCG NMC materials tested here did not seem to meet the target values. It was not clear what kind of concepts in terms of both compositional variations and process that will be tried this year.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer remarked that the potential high energy density of the system was very relevant to the DOE.

Reviewer 2:

The reviewer stated that higher capacity materials and cell designs were critical to the further adoption of electrified vehicles.

Reviewer 3:

The reviewer claimed that the work was directed towards achieving battery energy density targets for xEV.

Reviewer 4:

The reviewer said that high energy density materials and processes were important for meeting DOE's target goals for Li-ion battery technology.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer said that there were sufficient resources.

High Energy High Power Battery Exceeding PHEV-40 Requirements: Jane Rempel (TIAX) - es209

Reviewer Sample Size

A total of six reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that the approach of combining high energy cathodes and anodes together with electrolyte studies was very comprehensive. However, the authors were relying on experimental materials produced by others. The reviewer hoped that the quality and the reproducibility of those materials were good. The reviewer added that it was important for the authors to show data in larger cells, and that was clearly stated in the program and the results that were shown with the 18650 Li-ion cells.

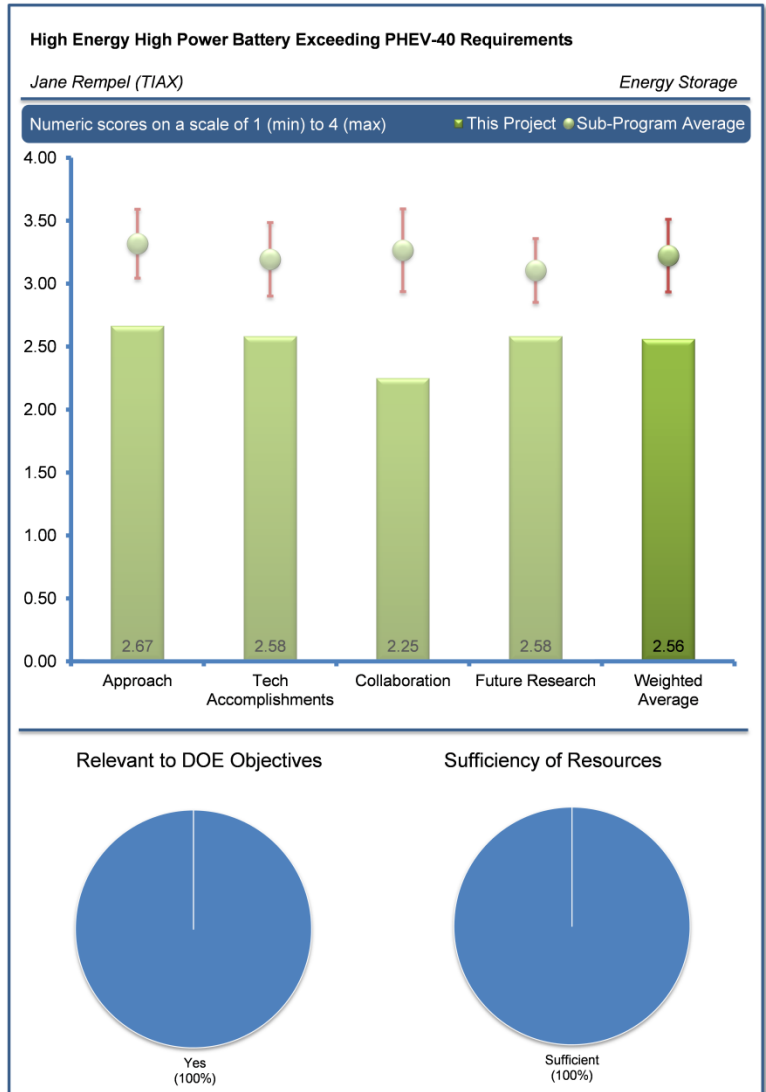
Reviewer 2:

The reviewer stated that it was very difficult to evaluate the validity and uniqueness of this project because there were not many technical details presented in either the slides or during the presentation beyond some general statements, such as using nano Si as anodes and separators with high porosity and thin thickness. The reviewer added that the slides and presentation raised many issues which may make the success of the project doubtful. Specifically, this reviewer is confused about the status of the “CAM-7TM High Energy High Power Cathode.”

It appeared to the reviewer, to be a unique and mature technology that satisfied the DOE requirements on Slides 5 and 6, but it became apparent on Slide 16 that the project would need to “explore cathode surface coatings” and “develop accelerated testing protocols” (see Slide 16), as well as to “continue cathode materials development to improve high temperature cycle life” and “down-select cathode formulation” (Slide 21). The reviewer wanted to know what was unique about CAM-7TM. The reviewer commented that it was unclear why “accelerated testing protocols” were needed because these have been developed by DOE labs as standard test procedures. Furthermore, the success of the project seemed to depend heavily on material suppliers (e.g., sourcing “several state-of-the-art silicon anode materials” (Slide 17) and accessing to “high purity electrolytes” and accessing to “production and research grade high performance separators ideal for energy and power applications” (Slide 19). However, the best industrial sources do not seem to have shelf-ready solutions as evident from the on-going DOE projects at various national laboratories on developing solutions to the same set of issues. This project can therefore have benefited from collaborations with national laboratories early on.

Reviewer 3:

The reviewer said that CAM-7/Graphite high energy 18650 cells showed stable cycleability up to 275 cycles, for commercial purpose 1000 cycle was necessary. The reviewer added that mass loading of anode electrode has a very big impact for high energy density and high power density for Lithium-ion battery. The reviewer said that this needed to be addressed.



Reviewer 4:

The reviewer indicated that the project made good attempts to use state-of-the art materials; however, it was difficult to identify the specialty or merits of this approach over others.

Reviewer 5:

The reviewer said that the approach was very difficult to assess from the presentation. The reviewer added that the focus on negative electrode properties and performance was not clearly stated. The importance of irreversible capacity was not discussed nor was the anode efficiency. The reviewer warned that without a careful assessment of these properties, a half cell assessment of the various supplier materials would not be predictable. Also, the method of mixing of hard carbon with silicon is not discussed, nor are the variations to be studied discussed. The reviewer commented that separator types were not discussed in the approach. Also, the reviewer said that electrolyte additive types were not discussed. Even though the cathode material had been available since at least 2010, few properties were disclosed in the presentation.

Reviewer 6:

The reviewer said that the development approach was not clear, where was it just a combination of the CAM7 material and other existing materials from material supplier. The reviewer stated that the interaction with partners for continuous improvement was not clear. The reviewer warned that relevant competencies to reach the target might be missing.

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.**Reviewer 1:**

The reviewer stated that there was decent progress in the initial stages of this project.

Reviewer 2:

The reviewer observed that the project had just started and that the authors had shown good progress. This project was important, in particular if the capacity fade, observed on the layered-layered materials, cannot be resolved or bypassed.

Reviewer 3:

The reviewer said that the cathode results still showed severe impedance growth in most coating formulations at 45 degrees. This result did not lead to any conclusions on the part of the presenter. The reviewer then remarked that indeed, it was not clear what the goal for the project was with regard to 45 degree cycling, so any result would be within the goals. High energy cells are only shown at room temperature, while high power cells are cycled at only current rate without any high rate pulse tests and only at 45 degrees. The reviewer added that anode testing had apparently just begun and properties such as irreversible capacity and anode efficiency are not presented. The reviewer said no information regarding the particular anodes tested was given. The reviewer stated that the baseline cell had only 1.9 Ah compared to the 2.7 Ah discussed in the introduction. The reviewer mentioned that no reason was given for the relatively poor performance of the baseline cell. The reviewer also commented that the separator work seemed to be rather limited. The reviewer added that no discussion of the use of coated separators for safety implementation was given.

Reviewer 4:

The reviewer remarked that the project was fairly new. The milestones have only been “scheduled” (see page 4). The reviewer pointed out that there was little information on the metrics used for “down select” Si and cathode formulation. The reviewer added that there was little information on how to “optimize electrode design in coin cells and select separator, electrolyte, cathode and anode formulations.”

Reviewer 5:

The reviewer commented that the interpretation of results was difficult due different testing protocols for different cell designs (e.g., 1,8 Ah cycling with 1C vs. 0,5C for 2,7 Ah). The reviewer added that the overall message regarding status of the work was not clear.

Reviewer 6:

The reviewer stated that using the state-of-the-art materials, the performance at a cell level appeared to be mundane and even inferior to the existing commercial products. The reviewer said that the capacity 1.9-2.7 Ah at C/20 for the 18650 form factor appeared to be surprisingly low compared to those of commercial products. The reviewer pointed out that this effort was supposed to be implementing the materials and developing state-of-the-art cells.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer stated that collaboration was only with suppliers of the materials. The reviewer added that the program would benefit from some collaboration with independent researchers. For example, many experts in cathode materials could provide valuable advice on the Cam 7 material and its use. Also, the reviewer claimed that many University and national laboratory people would be available to consult on anode effects and formulations.

Reviewer 2:

The reviewer reported that it should be beneficial to collaborate with DOE lab, especially on accelerated testing protocols. The reviewer also indicated that the project team had a heavy reliance on suppliers of Si, electrolytes, and separators, the project may not solve the challenges facing high capacity, high power, and long lasting lithium ion batteries.

Reviewer 3:

The reviewer did not see collaborators listed, and inquired if it was a trade secret or if there was no clue about what to do.

Reviewer 4:

The reviewer said that there was no obvious collaboration with partners, just material supply.

Reviewer 5:

The reviewer said that it was not very clear the collaboration the authors may have had with other institutions.

Reviewer 6:

The reviewer indicated that it was not clear about the collaborations and partners; no information was provided.

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.**Reviewer 1:**

The reviewer said that the third party verification of the main results, obtained by the authors, was highly recommended.

Reviewer 2:

The reviewer remarked that the direction of further development and improvement was not clear. The reviewer said that thermal stability and safety aspects should be included. The reviewer added that cost prognosis relative to state-of-the-art would be beneficial.

Reviewer 3:

The reviewer mentioned that no specific concepts were mentioned. It was difficult to evaluate the progress and future work.

Reviewer 4:

The reviewer observed that there was little information on how to quantify the success of proposed future work (page 21 and page 24).

Reviewer 5:

Nothing caught the reviewer's eyes.

Reviewer 6:

The reviewer reported that so few details were given regarding future work, that it was impossible to assess the program's future, the work will continue according to the presentation.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer indicated that the work was directed towards achieving battery energy density targets for xEV.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer was not sure but the project was big as far as the funding goes.

Advanced High Energy Li-ion Cell for PHEV and EV Applications: Jagat Singh (3M) - es210

Reviewer Sample Size

A total of seven reviewers evaluated this project.

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.

Reviewer 1:

The reviewer stated that the project was being carried out by an outstanding team from industry and government labs to overcome the main technical challenges facing high energy density and long cycle life lithium ion batteries.

Reviewer 2:

Just as the reviewer mentioned to other authors from a related project, the approach of combining high energy cathodes, anodes, together with electrolyte studies is very comprehensive. The reviewer said that it would be important to procure reproducible powder and electrolyte samples. The reviewer added that this project was very important, in particular if the capacity-fade observed on the layered-layered materials cannot be resolved or bypassed.

Reviewer 3:

The reviewer stated that the approach to high energy battery is based on improving the capability of the silicon anode for energy and stability as well as the capability of the high energy cathode, also with respect to energy and stability. This will require improvement in the anode binder, the cathode material, the electrolyte as well as processing improvements. The reviewer added that the approach to the anode binder is to take advantage of advances made by LBNL via the use of special electronically conductive binders, The approach to improving the electrolyte is to take advantage of improvements in voltage stability from ARL and 3M. The approach to improvements in processing is related to work carried out at Leyden Energy and scale up work at Umicore. The approach to improving the high energy cathode material is to utilize the 3M work on cathode composition variations to find optimum behavior. The reviewer commented that all of these steps are state-of-the-art and likely to yield progress in cell performance.

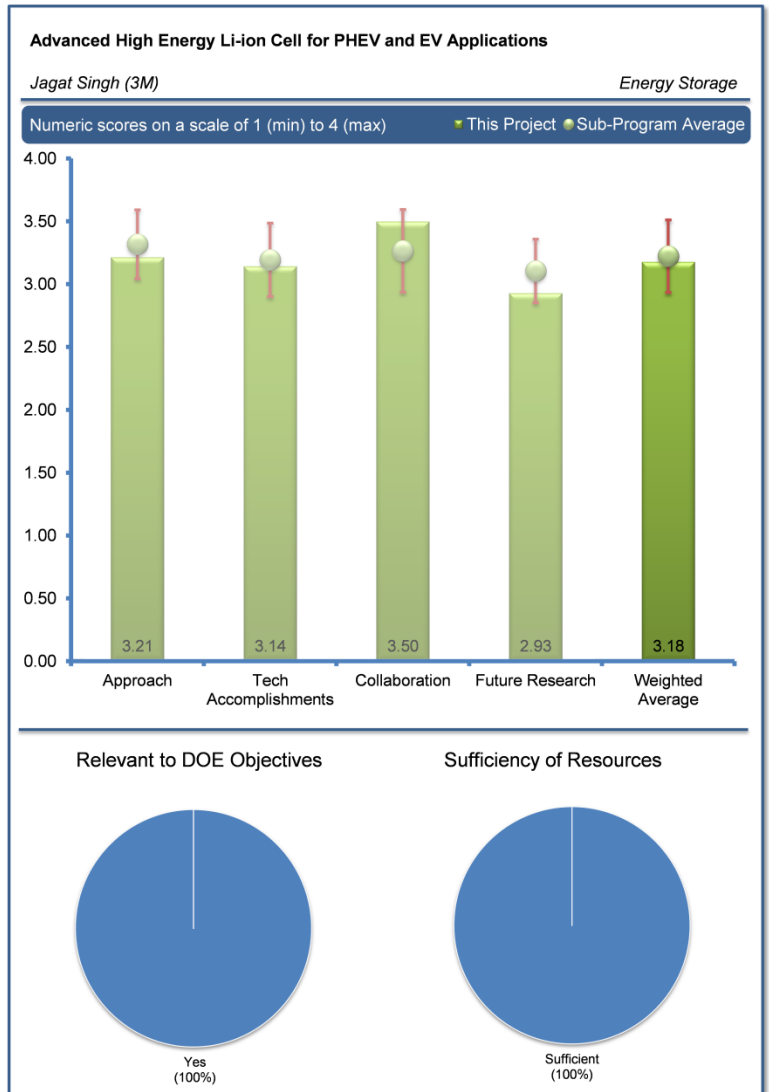
The reviewer indicated that the PI was using the best materials for both electrodes, fluoro-additives, and binder; these are great approaches. The reviewer asked what the project team got as a capacity or energy in the 18650 cells, rather than mAh/g, and suggested to provide form factor-based numbers. The reviewer observed that 3M has been working on both materials that were supposedly the state-of-the-art for quite a while. The reviewer wanted to know what has improved or achieved since 2-3 years ago.

Reviewer 4:

The reviewer indicated that the PI was using the best materials for both electrodes, fluoro-additives, and binder; these are great approaches. The reviewer asked what the project team got as a capacity or energy in the 18650 cells, rather than mAh/g, and suggested to provide form factor-based numbers. The reviewer observed that 3M has been working on both materials that were supposedly the state-of-the-art for quite a while. The reviewer wanted to know what has improved or achieved since 2-3 years ago.

Reviewer 5:

The reviewer explained that the general approach of developing a high energy anode, cathode and electrolyte system that work together was similar to the program being run by ANL. The reviewer said that specific technical barriers to success would need to be identified



more clearly and ways to address more clearly defined. The reviewer added that it was early in the program so the next review should focus on the clarity with these challenges that were identified and addressed.

Reviewer 6:

The reviewer said that discharge capacity versus cycle of Si alloy/NMC at the voltage range of 4.2-2.8 V at the C-rate of C/5 showed the capacity retention of 75%, improvement of capacity retention is necessary for commercial purpose. The reviewer added that mass loading of anode/cathode electrode full cell test also had a big impact on increasing the capacity and cycle life. The reviewer said that the author needed to focus on mass balance as well as electrolyte too. The reviewer indicated that volume expansion of silicon during the charge-discharge state is very severe up to 400% and capacity fades is also a big challenge. The reviewer observed that the author needs to focus on binder and Si alloy chemistry, too.

Reviewer 7:

The reviewer commented that the quantitative targets were not stated.

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.**Reviewer 1:**

The reviewer commented that the project just started and showed very good preliminary results.

Reviewer 2:

The reviewer noted that there were good accomplishments to date.

Reviewer 3:

The reviewer said that it was early in the program, and the establishment of the baseline performance seemed adequate.

Reviewer 4:

The reviewer indicated that the technical accomplishments were on material level progress in line with elapsed time since project start. The reviewer added that there were also technical accomplishments on cell level achievements in energy density, rate capability and cycle life quite far from target.

Reviewer 5:

The reviewer stated that the Leyden cell looked good. The reviewer also said that the NMC Scale up at Umicore appeared to be successful. The reviewer asked what the prospect was of achieving the 1000 cycle target. The reviewer also wanted to know why everybody was using Gao Liu's (LBNL) slide. Liu was everybody's partner and was used so many times to account budget although Liu has a DOE funded project. The reviewer asked if Liu's project was one effort for multiple credits.

Reviewer 6:

The reviewer stated that the target for developing Si alloy electrodes (e.g., 20% increase in mAh/g and 10% increase in mAh/cc) seemed achievable. The reviewer also said that the target for "high efficiency" and "surface stability" should be quantified. The reviewer added that modeling should include the coupled mechanical-chemical degradation mechanisms, especially since one of the members of the team, GM R&D Center, had published a number of papers in this field.

Reviewer 7:

The reviewer commented that the progress in the various steps was not exceptional in any property discussed above. The reviewer added that the high energy cathode variation had shown a slight improvement in capacity and first cycle efficiency at the C/20 rate for a new composition; however, the higher rate capacity was inferior to the older composition. This was not very useful, since the low rate was not usable in an electric vehicle. The reviewer also stated that the binder result was poor for silicon. The best reported LBNL binder was not tested and no explanation was given for this. The reviewer also said that the electrolyte result was also unimpressive with less than 200 cycles for the best result. Again, no explanation was given. The reviewer claimed that the cathode results were also unimpressive with increasing hysteresis over only 30 cycles, no explanation was given for this either. The reviewer mentioned that the electrolyte

additive result was rather poor. The reviewer was concerned about the lack of attention to these details and wonders how the team assesses results.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer explained that there was good collaboration with high competence. The reviewer added that fast progress should be expected if it is effectively coordinated.

Reviewer 2:

The reviewer reported that the project team was a strong multidisciplinary team with good credentials. The reviewer added that it was to the program's credit that a commercial manufacturer was developing the cathode material.

Reviewer 3:

The reviewer stated that there was good collaboration with other groups.

Reviewer 4:

The reviewer said that the collaboration was very extensive with a good prospect.

Reviewer 5:

The reviewer remarked that the project team had good collaboration with Industries, national laboratories and interaction with academia.

Reviewer 6:

The reviewer commented that the PI had assembled a very good team. The reviewer was concerned that the poor results of the first several quarters were an indication that the team was not functioning in a critical manner toward these results.

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.

Reviewer 1:

The reviewer mentioned that the approach of combining high energy cathodes, anodes, together with electrolyte studies was very comprehensive. The reviewer stated that it would be important to procure reproducible powder and electrolyte samples.

Reviewer 2:

The reviewer said that detailed identification of specific technical hurdles should occur as soon as possible with focus on these going forward.

Reviewer 3:

The reviewer reported that the strategy to improve cell performance was not fully clear. The reviewer suggested that the thermal stability and safety aspects should be included. The reviewer added that the cost prognosis relative to the state-of-the-art would be beneficial.

Reviewer 4:

The reviewer stated that the details were not sufficiently provided to analyze future work.

Reviewer 5:

The reviewer asked that the presentation team show the 18650 data. The reviewer suggested that the project team tell the prospect of achieving 1000 cycles next time.

Reviewer 6:

The reviewer cannot evaluate because of lack of detail. The reviewer added that there seemed to be a poor sense of detailed direction.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer stated that high energy electrode materials and cell designs are critical to electrification of vehicles at any level.

Reviewer 2:

The reviewer said that this project was relevant to advance commercial implementation of high energy density Li-ion battery technology.

Reviewer 3:

The reviewer mentioned that the work was directed towards achieving battery energy density targets for xEV.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that all relevant resources appeared to be available to the team.

High Energy Lithium Batteries for PHEVs: Subramanian Venkatachala (Envia) - es211

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer asserted that this project is important and very challenging. As mentioned by the authors, the main problem with the cathode powder is the capacity fade observed with the layered-layered materials. The commenter highlighted that the mitigation strategies are showing some promising results such as the coating developments.

Reviewer 2:

The reviewer stated that the targets were clearly defined in detail and that the approach to meet the targets was well structured.

Reviewer 3:

The reviewer pointed out that the author mentioned that high capacity Mn rich $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$ cathode electrode showing the capacity of 240 mAh g⁻¹ at C/10 at the voltage range of 4.6-2.0V, which is good for high energy density. The reviewer added that the project team did not show more cycles of charge-discharge curve of Mn rich $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$ cathode electrode because there is a high chance of layered Mn rich $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$ cathode electrode to change into spinel phase at high voltage test. The reviewer also said that a PHEV cell with high capacity manganese rich (HCMR) XP cathode shows 75% capacity retention up to 5000 cycles, which is good for commercial application. The reviewer also said that the author mentioned that nano coating can improve the capacity increase up to 15 mAh g⁻¹ but, ALD coating of Al₂O₃ and AlF₃ shows the similar performance like the pristine electrode. The reviewer asked how the ALD coating can help with high voltage cell tests.

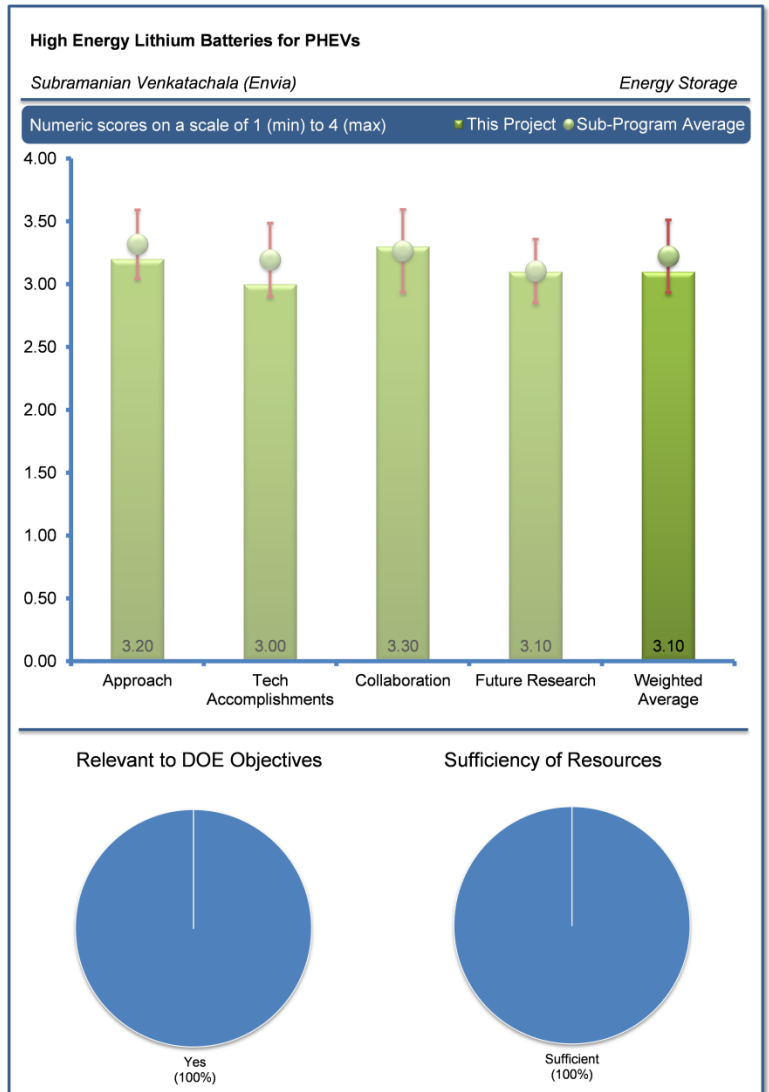
The reviewer also said that a PHEV cell with high capacity manganese rich (HCMR) XP cathode shows 75% capacity retention up to 5000 cycles, which is good for commercial application. The reviewer also said that the author mentioned that nano coating can improve the capacity increase up to 15 mAh g⁻¹ but, ALD coating of Al₂O₃ and AlF₃ shows the similar performance like the pristine electrode. The reviewer asked how the ALD coating can help with high voltage cell tests.

Reviewer 4:

The reviewer asked why there were such large form factor cells. The reviewer explained that larger cells were believed to have more issues than advantages (e.g., defect probability, maintenance cost, thermal managing, etc.). The reviewer stated that lithium phosphorous oxynitride (LiPON) coating sounded very expensive. The reviewer wanted to know if it could be cost effective, which was one of the critical barriers.

Reviewer 5:

The reviewer said that the approach is to improve the baseline cathode material from Envia, which is different from ANL material (Envia has licensed the ANL patents) in unspecified ways. The reaction mechanism under charge at high voltage is alleged to be Li₂MnO₃ going to MnO₂, lithium ions and oxygen. The reviewer added that this proposal is obviously a great simplification. If true, the MnO₂ that is cycling would be transformed completely to spinel material with gradual loss of capacity and substantial loss of voltage. Further



improvement is sought by coating the active material with various coatings and various methods. Also, the reviewer stated that there is a lot of information regarding coatings already in the literature, but no effort is made to distinguish their approach from work already done. The reviewer indicated that various partners and Envia will carry out the coatings consisting of LiPON, polymers, conductive and nonconductive, ceramics, and carbon. The reviewer also reported that silicon anodes will be made with Envia prepared silicon and LBNL electronically conductive binders. The reviewer commented that the approach to ranking the various coating types and experimental protocols to evaluate the many coatings is not specified. The reviewer finds this troubling and will detract from the program if the work is not done according to some systematic planning. The reviewer noted that the PI suggested that the project team may investigate doping of the cathode material in order to minimize voltage fade. The PI also states that one of the forms of Envia HCMR material has no voltage fade. The reviewer is suspicious of such contradictory claims. The reviewer asked if there was no voltage fade, why the project team needed to study doping.

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.

Reviewer 1:

The reviewer commented that there was significant progress to date.

Reviewer 2:

The reviewer remarked that status was shown on relevant cell size and that reasonable test conditions results were very valuable.

Reviewer 3:

The reviewer said that the project has just started. The reviewer added that, in the future, it is going to be important to clearly propose mitigation strategies in case the capacity fade of the HCMR cathode layered-layered materials cannot be resolved. Also, the reviewer stated that the atomistic model, suggesting Mn migration to the Li layer is important. Additionally, the reviewer suggested that it could be of great interest to study that mechanism further so that solutions or partial mitigation strategies can be proposed.

Reviewer 4:

The reviewer commented that Envia is supposed to integrate cells rather than to carry out material studies. The reviewer noted that there was too much characterization data. The reviewer would like to see more cell trial data.

Reviewer 5:

The reviewer stated that it was somewhat difficult to understand what had been accomplished with this program and what refers to prior work. The reviewer added that three different morphologies of cathode active material had been discussed, but it was possible that all these materials were already available. The reviewer said that this extended to the carbon coating work as well. The ORNL coating of LiPON did appear to have been carried out in this program. The reviewer noted that the results of LiPON coating were not as good as the carbon coating where the voltage fade was worse and the capacity was lower. No explanation was given for this result. It is important to assess the work as it continues, particularly when so many coatings are planned and poor results should not be pursued. The ALD coatings showed comparable results on voltage fade compared to carbon coatings, but poorer results on capacity. Again, no conclusions were drawn. The reviewer pointed out that only one slide was devoted to anode development and that said that LBNL binders would be employed. Apparently, no work was done on this aspect.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer reported that the project team had good collaboration with national laboratories and industry.

Reviewer 2:

The reviewer commented that the project was well structured and that work packages were clearly addressed to partners.

Reviewer 3:

The reviewer stated that the collaboration looked good.

Reviewer 4:

The reviewer stated that the collaboration and coordination seems to be very good.

Reviewer 5:

The reviewer said that it was not clear that good communication among the many partners had been established. The reviewer added that on paper it looked good, but if there was not an effort to communicate results and do team evaluations of results, the program was unlikely to succeed.

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.

Reviewer 1:

The project has just started. As mentioned earlier, in the future is going to be important to clearly proposed mitigation strategies in case the capacity fade of the HCMR cathode layered-layered materials cannot be resolved. The reviewer suggested that it could be of great interest to know how reproducible are the HCMR powders used by the authors in this study. The commenter also pointed out that the Si-C based anode is also becoming increasingly more complex. The reviewer recommended that the authors should focus also on the reproducibility of their results.

Reviewer 2:

The reviewer stated that the approach on modeling combined with experiments for their proposed concepts of using nano-coatings seemed reasonable.

Reviewer 3:

The reviewer remarked that the modeling should be extended to the effect of doping und compared to experimental results. Also, the reviewer said that thermal stability and safety aspects should be included. The reviewer added that the cost prognosis relative to state-of-the-art would be beneficial.

Reviewer 4:

The reviewer asked if the project team would like to test smaller cells as well, or if developing large cells itself was the goal of the project.

Reviewer 5:

The reviewer stated that the future work plans were extremely broad and do not form the basis for the evaluation. The reviewer reported that the project team basically said that the work would continue. In fact the plans to do extensive studies of LiPON coatings did not make a lot of sense to this reviewer as they are clearly inferior in properties studied to date to the carbon coating and no known method existed to make an economically viable coating of this material.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer claimed that the relevance would be sacrificed if good planning was not applied to this program.

Reviewer 2:

The reviewer stated that the work is directed towards achieve battery energy density targets for xEV.

Reviewer 3:

The reviewer commented that just like many other projects, high energy density and durable electrode materials were necessary for meeting DOE's targets for Li-Ion battery technology toward electric vehicles.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

No comments were received in response to this question.

High Energy, Long Cycle Life Lithium-ion Batteries for PHEV Applications: Donghai Wang (Pennsylvania State University) - es212

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer indicated that this project was very important, in particular if the capacity fade observed on the layered-layered materials cannot be resolved or bypassed. The reviewer added that it was not very clear if the authors were using a two layer powder, as a cathode powder, with two clear compositions, or a gradient powder. The first will have a Ni-rich core surrounded by a Mn rich outer layer. A gradient powder will have a Mn outer layer that gradually changes in composition with higher Mn content looking towards the surface of the particle.

Reviewer 2:

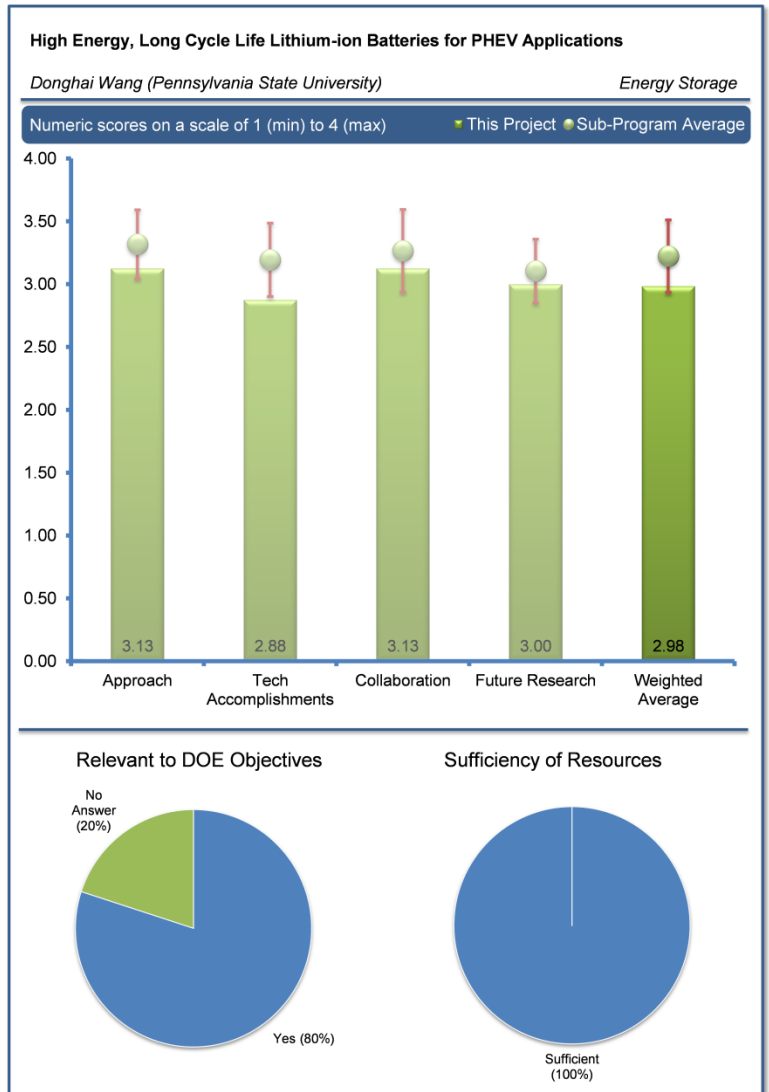
The reviewer commented that the approach was much more academic than alternate programs, with more focus on individual components rather than a coordinated activity. The reviewer added that individual component advances could occur; however, integrated performance demonstration was less likely.

Reviewer 3:

The reviewer stated that the author showed micro size Si-porous C anode electrode showing high capacity of 2400 mAh g⁻¹ up to 50 cycles. The reviewer explained that it was not clear on what strategies were implemented for minimizing the first irreversible capacity loss. Also, the reviewer said that it was mentioned that the fluorinated electrolyte additive enable higher capacity at 4.8V to achieve high energy density but, the capacity fade was also a big problem. It was not clear on the proposed solution. Additionally, the authors mentioned developing cathode materials but no new ideas or concepts were proposed.

Reviewer 4:

The reviewer stated that the cathode material of Ni-rich core and Mn-rich shell looked good. The reviewer asked how this compared with the ANL material. The reviewer also wanted to know if this Si-C composite was superior to those from 3M or Amprius. The reviewer suggested that the project team show some comparison to these other materials, and was always good to show advantages and superiority over the existing competitor or the state-of-the art. The reviewer added that the functional binder sounded good; however, it was led by those at LBNL who have their own project. That effort should not get multiple credits or other party additions to own project to get a credit. The reviewer queried what was special about the project team's fluorinate electrolyte, and whether this was fashion.



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.

Reviewer 1:

The reviewer asked what accomplishments belonged to the project team and what accomplishments belonged to collaborators who have their own projects. The reviewer said to see the comments above.

Reviewer 2:

The reviewer indicated that the project had just started and that the authors had shown good progress.

Reviewer 3:

The reviewer stated that the materials capability had been base-lined, but it was not clear that an integrated baseline cell structure had been developed and characterized.

Reviewer 4:

The reviewer remarked that the technical accomplishments with the anode seemed good, but that the progress with cathode did not seem to be as good.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team had good collaboration with industry and national laboratories.

Reviewer 2:

The reviewer said that the collaboration and coordination looked good.

Reviewer 3:

The reviewer stated that the collaboration seems to be good; however, the reviewer suggested that it may be too early to tell.

Reviewer 4:

The reviewer commented that collaboration groups appeared to be competent. The reviewer pointed out that the presenter was far less informed on the work occurring at the collaborators than other program presentations.

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.

Reviewer 1:

The reviewer said that this project was very important, in particular if the capacity-fade observed on the layered-layered cathode materials cannot be resolved or bypassed. The reviewer suggested that the scale up of the anode and cathode materials should be better clarified.

Reviewer 2:

The reviewer thought that the project team should consider benchmarking with other materials.

Reviewer 3:

The reviewer commented that the proposed studies on first cycle efficiency for silicon anode were important. The reviewer added that it seemed that the proposed studies were scattered and were not focused enough to warrant significant progress within the project duration.

Reviewer 4:

The reviewer said that the program seemed perhaps less integrated into the much more integrated set of programs otherwise presented in this section. This was just an observation, without any further insight.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

No comments were received in response to this question.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

No comments were received in response to this question.

High Energy Density Li-ion Cells for EVs Based on Novel, High Voltage Cathode Material Systems: Keith Kepler (Farasis) - es213

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer observed that the targets were clearly defined in detail and that the approach to meet the targets was well structured.

Reviewer 2:

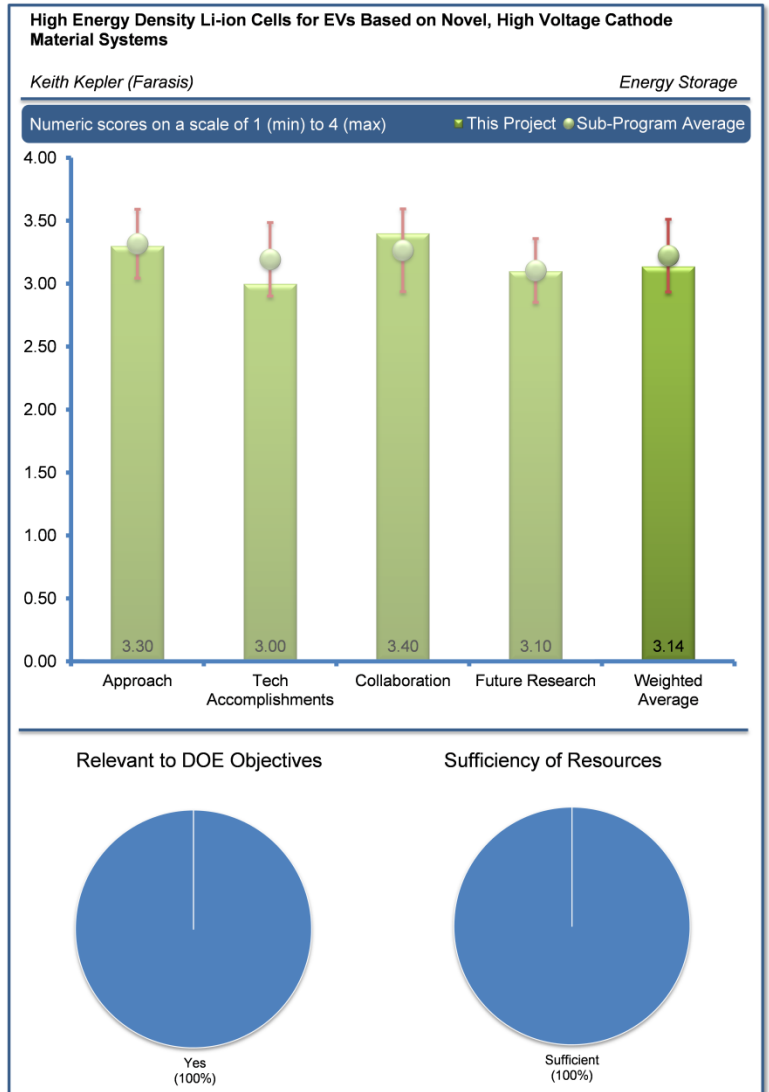
The reviewer reported that the approach of combining high energy cathodes, anodes together with electrolyte studies was very comprehensive. It will be important to procure reproducible powder samples. The reviewer added that it was important to produce generation one cells with a more traditional anode, so that it can be used as a baseline.

Reviewer 3:

The reviewer commented that the approach was to develop cells with lithium and manganese rich cathode materials containing cobalt, derived from ion exchange process (sodium to lithium). This was known to produce stacking faults and some spinel content in addition to the layered-layered structure. The reviewer added that this type of material was known to have better stability in cycling and is capable of higher power than the standard layered-layered structure material. The reviewer stated that this work was done in collaboration with ANL. A second cathode approach was to investigate stoichiometric NCM materials doped with other transition metal ions, which have a coating to stabilize the material to high voltage. The reviewer also said that the coating technology is supplied by LBNL. The reviewer added that the second strategy was to use a silicon anode material derived from silicon whisker growth directly on carbon developed by Nano-system and currently supplied by OneD Material LLC. This material has displayed good power capability and high efficiency. The reviewer also remarked that the third aspect of the approach was to utilize stabilized electrolytes and separators developed at DuPont, which continues to work on developing new materials and supplies the PI. These aspects were all addressing the barriers that have been encountered in earlier work regarding high capacity, high voltage materials.

Reviewer 4:

The reviewer stated that if the assumption is followed, ion exchange (IE)-NCM is supposed to be more stable at higher voltages. The reviewer wondered if the experiments supported this. The reviewer stated that the capacity fading was significant at 4.6V. The reviewer wanted to know if the project team was planning to compare “usual” NCM and IE-NCM after doping. The reviewer then inquired about the target performance, volumetric energy, as well as power and number of cycles for the pouch and 18650 cells.



Reviewer 5:

The reviewer stated that the author shows the cycle performance of NCM(532) cathode electrode at high voltage of 4.6 V to achieve high capacity more than 200 mAh g⁻¹, but the capacity fading after 50 cycles was nearly 60%. The reviewer added that the selection of a moderate voltage was necessary. Also, the reviewer said that the ion exchange layered lithium (LL)-NCM showed stable capacity of over 200 mAh g⁻¹ at the high voltage range of 4.7-4.9-2.0V up to 20 cycles.

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.**Reviewer 1:**

The reviewer stated that there were substantial and meaningful results. The reviewer added that the capacity and energy density of baseline cell was quite low taking into account the use of LL-NCM.

Reviewer 2:

The reviewer remarked that the project had just started and that the authors had shown good progress.

Reviewer 3:

The reviewer stated that the baseline cells involving LL-NMC/graphite cells had been supplied to INL and that test protocols had been developed. The reviewer added that the 18650 cylindrical and pouch cells had been designed for electrolyte developing using experimental electrolytes as well as separators in a first round study at 4.4 and 4.6 V. The cells use conventional NCM and graphite. This appeared to be a good couple to study electrolyte problems. The reviewer stated that silicon anodes would also be incorporated into this work. Unfortunately, no details regarding the electrolytes under study have been supplied. The reviewer would like to see such information to assess the likelihood of success of this work. Also, the reviewer said that the stabilized NCM had been received and preliminary evaluation was carried out. Early cycling data at 4.6 V appeared promising. Silicon anode material had also been received and preliminary evaluation carried out. The reviewer said that only about 600 mAh/g was achieved and the cells faded in capacity over 150 cycles. This relatively poor result was a concern for anode progress. Finally, the reviewer noted that the ion exchange derived LL-NMC was tested and early cycling appeared promising although some power fade was already apparent.

Reviewer 4:

The reviewer commented that the project team should show actual numbers in the capacity instead of normalized values. The reviewer noted that it looked like cells were being built. The reviewer asked if the project team would share the actual performance data.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer commented that the project team has good collaboration with industries and national laboratories.

Reviewer 2:

The reviewer said that the collaboration and coordination looked good.

Reviewer 3:

The reviewer stated that the project was well structured and work packages clearly addressed to partners.

Reviewer 4:

The reviewer indicated that the collaboration seems to be good; however, the reviewer suggested that it may be too early to tell.

Reviewer 5:

The reviewer indicated that collaboration with ANL, LBNL and DuPont all appeared to operate at good levels. The reviewer said that the collaboration with OneD appeared to exist, but the poor results with initial materials may be cause for concern.

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.

Reviewer 1:

The reviewer commented that the future work plans were solid. The reviewer added that the continued work on silicon anode should have a high priority, as preliminary work was not good enough for long term cycling.

Reviewer 2:

The reviewer explained that the use of pouch cells and 18650 was important. The reviewer added that the authors should make efforts to fully characterize the cathode and anode powders to make sure that the results are reproducible. The reviewer stated that these experimental materials were not easy to synthesize in large amounts.

Reviewer 3:

The reviewer indicated that a decision matrix and key performance indicator to decide between the two cathode material options should be clearly defined. The reviewer said that thermal stability and safety aspects should be included. The reviewer added that a cost prognosis relative to state-of-the-art would be beneficial.

Reviewer 4:

The reviewer reported that the proposed research involved stabilization of high voltage cathode materials using dopant additions. The reviewer added that it was not clear on how they would be chosen and added to the materials structures.

Reviewer 5:

The reviewer suggested that the project team show benchmarking data with respect to non-IE materials not normalized data but raw data. Then the reviewer said that the project team should set cell performance targets and show the progress by the data.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer stated that the work was directed towards achieving battery energy density targets for xEV.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

No comments were received in response to this question.

First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anodes: Perla Balbuena (Texas A&M University) - es214

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer was very glad to see a theoretician study the SEI layer working with experimentalists who are specialized in electrolytes and SEI layers. The reviewer added that it was not clear how the surface of Si was treated as the initial state and structure. The Si surface often terminated by oxides before lithiation, thus, it would be covered by Li_2O when lithiated. The reviewer asked how that would affect the simulation.

Reviewer 2:

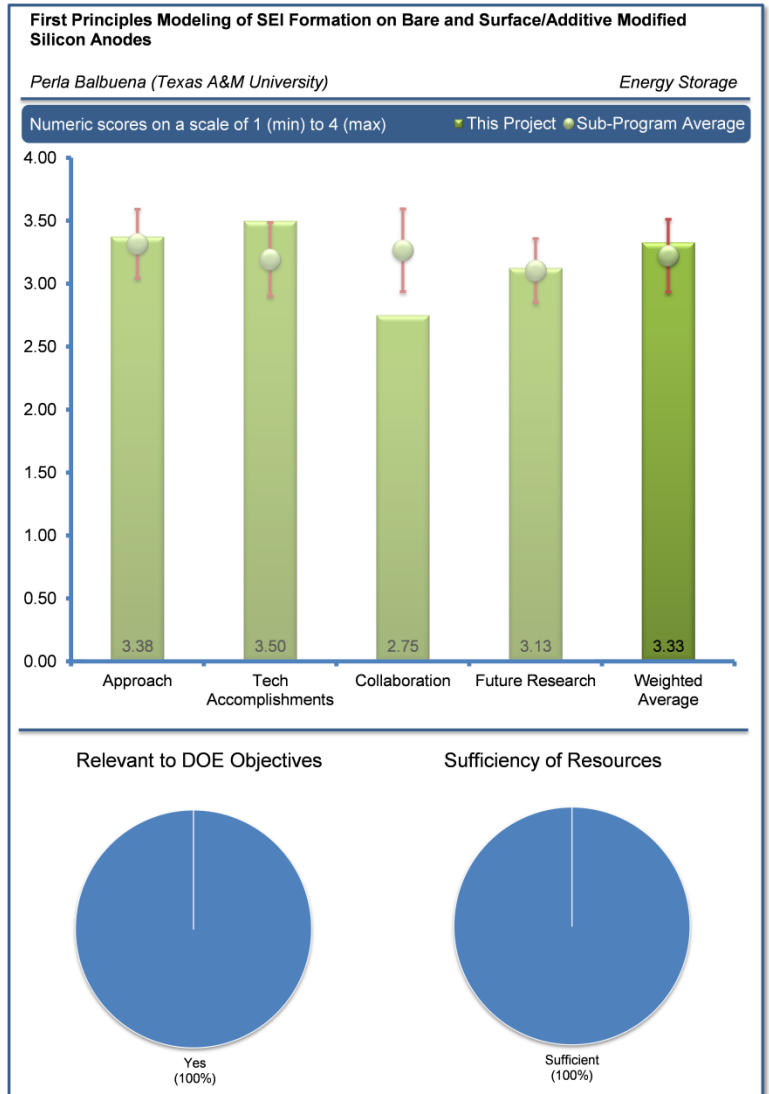
The reviewer stated that the project had a good, from the beginning, modeling approach in that the project team was factoring in the actual electrode surface in the reaction that includes steric effects as well as energetics. The reviewer reported that it seemed rigorous, but the reviewer really did not have the expertise to determine that. The reviewer indicated that this project seemed to be an improvement on the work done a few years ago at the University of Utah. The reviewer suggested that the project team asked University of Utah to critique this work offline (e.g., Oleg Borodin now at the U.S. Army Research).

Reviewer 3:

The reviewer's limited experience with first-principles calculations of interfaces is that they are quite challenging. The reviewer added that taking on the SEI formation of a phase-change negative electrode is carving out a very difficult problem. The reviewer stated that the PI's approach, to developing the active material models then exposing the active material to various solvent molecules, seems good. Also, the reviewer said that the issue when building the SEI is how idealized it has to be and whether it is realistic or not.

Reviewer 4:

The reviewer commented that this modelling program investigates the surface structure of silicon lithium alloys, the interaction of electrolyte solvent, salt with the surface and the reactions of electrolyte with the surface to form a solid electrolyte interface with the reaction products, all at various stages of lithiation of the surface, from four different lithium silicon alloys. The reviewer added that the properties of the SEI will be studied to help interpret the effect of capacity loss and SEI growth as the electrode is cycled.



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.**Reviewer 1:**

The reviewer indicated that four important milestones have been achieved since the start of the program. The first is that the most favorable surfaces of the alloys have been determined and their reactivity characterized. The second is that a preliminary model of the SEI and its thickness has been established. The third is that surface effects for solvent component reactivity have been studied including solvent decomposition. The fourth is that reaction pathways and activation energies for ethylene carbonate (EC) and fluorinated ethylene carbonate (FEC) have been identified. The reviewer explained that this has been a substantial accomplishment and sets the stage for developing the model for SEI growth as well as capacity fading with cycling. The reviewer hopes that the study will point the direction toward improved electrolytes.

Reviewer 2:

The reviewer said that overall, the results seemed consistent with the experiments. The reviewer added that the solvent and additive molecule reactions seemed to have a lot of two electron reductions, which seems unusual. The reviewer especially liked the PI's observations about FEC.

Reviewer 3:

The reviewer indicated that the reaction of lithiated Si surfaces with the solvent looked good. The reviewer asked if the project team had experimental confirmation for the given reaction mechanism or reaction products.

Reviewer 4:

The reviewer observed that the project shows the degradation reaction mechanism of EC and FEC. The reviewer commented that there was nice work showing that both FEC and VC, which both increase cell cycle life and stability, react to give the same surface species. The reviewer was very supportive of this from the beginning work as it provides insight that is hard or impossible to get experimentally. In addition, the reviewer said that the project team can go back into their models and explain why certain reactions are preferred, not just identify the reaction products. Doing this experimentally, if it were possible, can provide a more accurate estimate of what is actually formed, but leads one to infer the mechanism. Understanding the mechanism, which modeling can help provide, could be critical in trying to design an interface and SEI layer and provide direction to new solvents and salts.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer reported that the Collaboration for the most part was excellent; however, the contract has not been completed for the collaboration with SNL as yet. The reviewer added that this was an important part of the program as substantial parts of the computations were planned to be carried out at SNL and it is necessary to complete these negotiations in order to reach the goals of the project. If the agreement is not reached, a modification of the contract with DOE may have to be agreed upon.

Reviewer 2:

The reviewer stated that there was a great combination with experimentalists who have focus on electrolytes and SEI layers.

Reviewer 3:

The reviewer stated that the PI has established a few collaborations. The reviewer thought that the PI was smart to team with experimental efforts to support the work.

Reviewer 4:

The reviewer commented that the work desperately needed validation by experimentalists. The reviewer suggested that the project team link up Sommarjai/es215 work where the project team was using FTIR to study surfaces and get at organic structures formed on the electrode surfaces on site.

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.

Reviewer 1:

The reviewer noted that it would be nice to see the ion conduction mechanism in the SEI layer, identifying any limiting factors in the diffusivity, which would guide the electrolyte optimization.

Reviewer 2:

The reviewer observed that the proposed development of the SEI model would allow modelling of the nucleation and growth of the SEI, the electronic and ionic conductivity of the SEI and the effect of voltage on these properties. The reviewer said that these would then lead to a mesoscopic model of the SEI which can be compared with experiment. The reviewer added that the aspect of prediction of solvent types for superior SEI properties should be an important goal of this part of the project.

Reviewer 3:

The reviewer remarked that the PI's focus for the future is to build up her SEI model. Again, this was quite challenging and interesting. The reviewer added that there did not seem to be any effort to improve the interface, such as predicting better additives.

Reviewer 4:

The reviewer indicated that the project needs better collaboration to get validation of their modeling results. The reviewer said that plans to look at follow on reactions to form complete SEI should provide good fundamental knowledge. The reviewer suggested looking at the fluorinated ethers being developed to improve cycle life. Also, the project team should, if possible, model a mixed solvent electrolyte system and salt. The reviewer pointed out that modeling new solvents to guide the partner's ability to design new solvents for Li-Ion cells is a laudable goal. The reviewer was not sure if this work could really do that, but maybe a better understanding of the existing SEI formation process could provide direction.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer commented that the project was addressing SEI formation and could lead to new electrolytes that give more stable SEIs and improve cycle life of new high energy density cells using silicon anodes.

Reviewer 2:

The reviewer reported that the PI did not make the best case for relevance, but developing an alloy based negative electrode would greatly improve lithium-ion battery technology.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer said this may depend on the agreement with SNL.

Reviewer 2:

The reviewer stated that there are sufficient funds to conduct the studies based on the PI's productivity.

Reviewer 3:

The reviewer said that the project team needed a partner or more help from others in the program.

Analysis of Film Formation Chemistry on Silicon Anodes by Advanced In Situ and Operando Vibrational Spectroscopy: Gabor Somorajai (University of California, Berkeley) - es215

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer noted that surface vibration spectroscopic probes are powerful to collect molecular specific information for SEI films. However, it would be nice to show the electrochemical cell setup. The reviewer added that to enhance the sensitivity, excitation of surface plasmon using a Kretschmann configuration was a very good approach. The reviewer asked why the gold “electrode” was necessary. To excite plasmon, the gold film on the internal reflection element need not be electrically connected. To observe the SEI film formation on silicon (Si) in the vicinity can cause gold-lithium (Au-Li) alloy formation, which causes the optical property changes including the plasmon excitation angle, likely leading to modulation of spectral features. The reviewer acknowledged that the University of California-Berkeley is the birth place of vibrational sum frequency generation (SFG) (R. Shen’s in late 1980’s). The reviewer asked how to do SFG on Si nano-particles. SFG requires mirror like surfaces to detect coherent signals. The reviewer then asked if there were any preliminary results.

Reviewer 2:

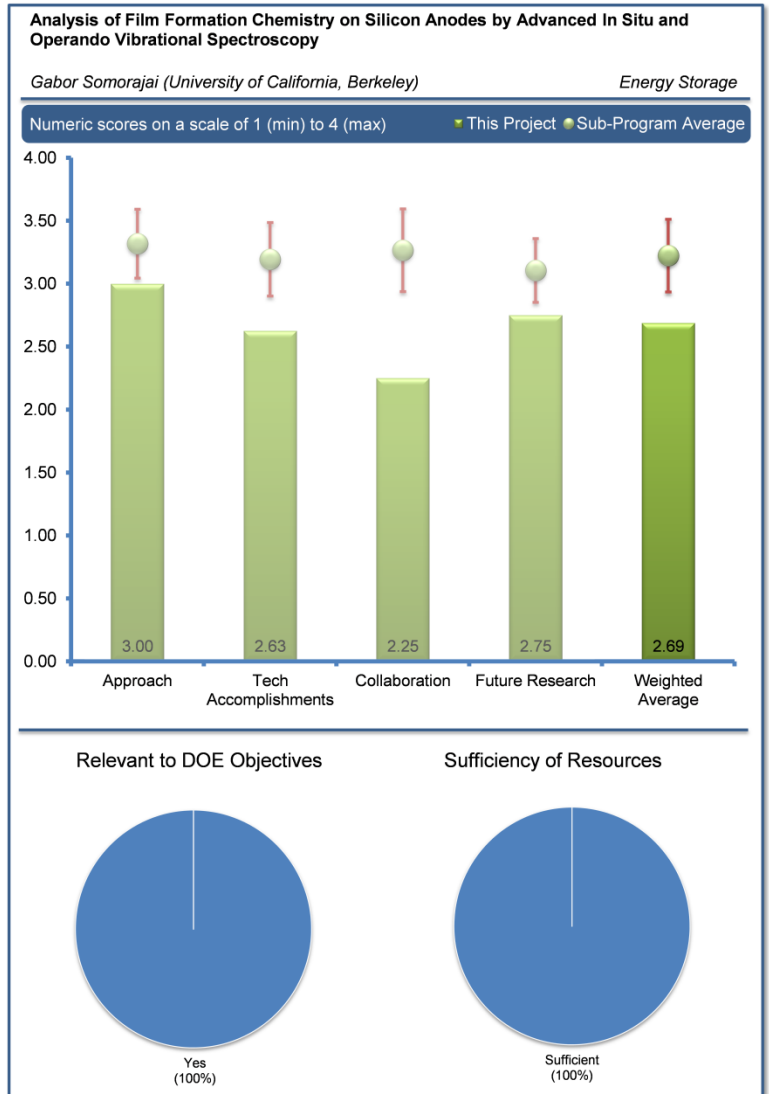
The reviewer noted that attenuated total reflection (ATR) in combination with stem to develop high spatial resolution of the SEI on various materials shows promise to achieve additional information regarding the SEI. This can be useful in solving problems related to high energy anodes as well as reaction products formed on high potential cathode materials.

Reviewer 3:

The reviewer said that the PI used a non-standard format for his poster presentation. As a poster this was fairly well laid out, but for the purposes of this review, the PI should have submitted the work in the standard format.

Reviewer 4:

The reviewer said that FTIR or surfaces in the electrolyte by passing a beam from underneath the electrode. The reviewer noted good use of angle to vary sample depth and differentiate between bulk and surface films. The reviewer commented that the presentation was very sparse (one slide) and that more detail would have been better to review this project.



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.**Reviewer 1:**

The reviewer said that the PI had some interesting results, but the project appeared to be in its early stages.

Reviewer 2:

The reviewer noted that the material indicates that the new in situ ATR -FTIR cell was developed, but it is not clear if this was done as part of the contract or existed previously. The detection of soluble dioxohexane dicarboxylate (DEDOHC) on Si and tin surfaces could be a useful result.

Reviewer 3:

The reviewer observed signs of DEDOHC on the surface. However, the reviewer felt that the known reactions of EC and DEC during formation to form DEDOHC in the liquid electrolyte were not appreciated. This reaction, along with transesterification when more than one dialkylcarbonate is present, is pretty well-known. The reviewer indicated that Kerr, et. al., published papers on this, and provided the following references: J. Power Sources (2003) 119-121, 330; and Electrochem. Solid State Lett.,(2001) 4, A42. The reviewer then noted that the project pointed out only seeing this at the surface, but the interactions between the two solvents was important. The reviewer recommended checking the liquid phases by GC to really differentiate between reactions at the surface and reactions that can occur in the bulk initiated by alkoxide ions generated at the surface from EC degradation.

Reviewer 4:

The reviewer inquired about spectral analyses.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer said that the collaborations seemed rather limited, but that it was difficult to determine from the presentation.

Reviewer 2:

The reviewer commented that the collaborations were not discussed, but should be encouraged to ensure that important problem areas are pursued.

Reviewer 3:

The reviewer noticed that the presenter seemed to be completely disconnected from the rest of the DOE program.

The reviewer noted that this work needed to be closely linked with the modeling work (e.g., es214). Also, the reviewer asked if there had been talks with John Kerr at Berkeley about this work.

Reviewer 4:

The reviewer asked that the presentation please list collaborators. Both PIs are not known for surface vibrational SFG.

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.**Reviewer 1:**

This reviewer looked forward to some more results.

Reviewer 2:

The reviewer commented that the proposed future research was only sketched out. Indications were given that FEC would be studied and surface modifications of Si, would be tested, although the type of modification was not mentioned.

Reviewer 3:

The reviewer noted that there were only a couple of statements on the future work and that it was difficult for the reviewer to determine the overall plan for the project.

Reviewer 4:

The reviewer said that the plan was to look at FEC next, which seemed reasonable. The reviewer added that it might be good to look at other salts maybe and/or VC. The reviewer's main problem with the future plans was the disconnect between this and modeling work – both present and past work.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This reviewer commented that this work is very relevant for the advancement of lithium-ion battery technology.

Reviewer 2:

The reviewer stated that the SEI layer is still very poorly understood and that this method could provide valuable insight.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

This reviewer stated that UC Berkeley is self-sufficient for this project assuming the Department of Physics folks who are specialized in SFG are available. The reviewer thought both PIs were retired and was glad that both were active.

Reviewer 2:

The reviewer said that it was difficult to determine this accurately, but had the impression that the funds were adequate.

Reviewer 3:

The reviewer thinks that this PI and postdoc needed a lot of help. The reviewer added that the PI and postdoc seemed to be working in isolation from others.

Optimization of Ion Transport in High-Energy Composite Cathodes: Shirley Meng (University of California, San Diego) - es216

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

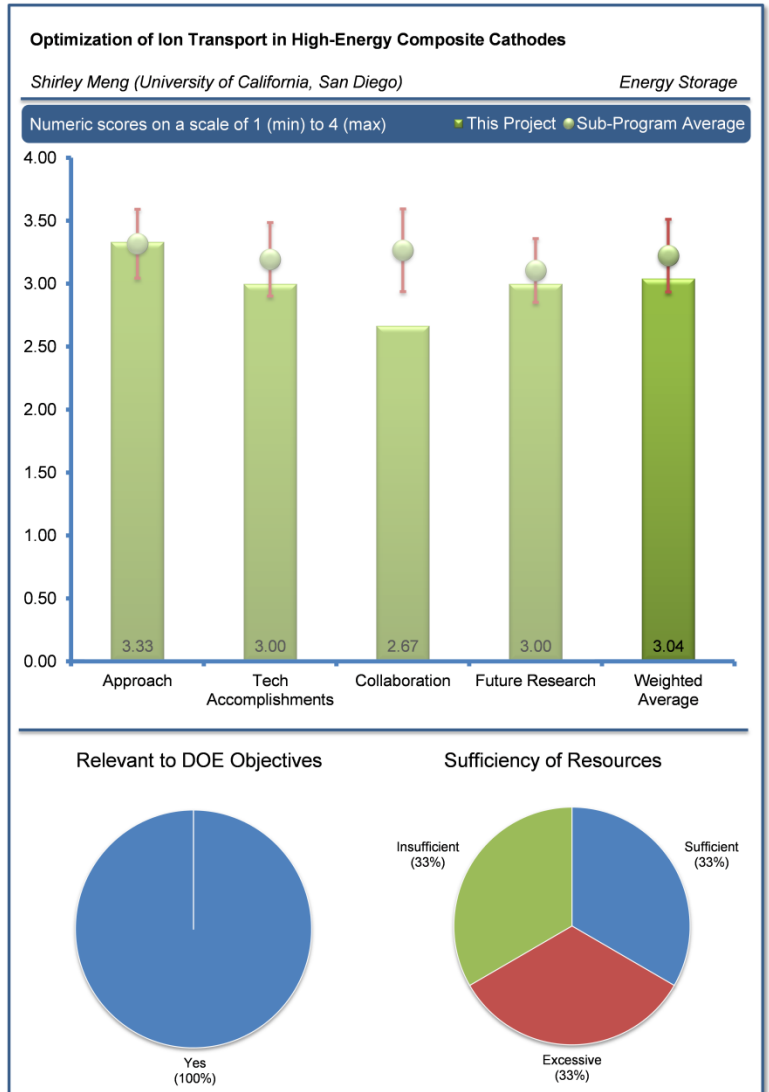
The reviewer commented that the high energy cathode material that the PI refers to actually has a very wide compositional range and very complicated property/composition/structure relationships, making any study of this material challenging. The PI's approach of doing a wide range of diagnostic studies, combined with synthesis and first-principal calculations, to examine these cathode materials is good. However, the reviewer added that it does run the risk of being too wide and shallow, creating an increased possibility of making preliminary conclusions that are not fully substantiated.

Reviewer 2:

The reviewer noticed that the approach to this work builds on the expertise of the PI in the fields of electron and X-ray absorption and scattering experimentation at the scale of atomic resolution to characterize the surface as well as the bulk structure effects for materials of greatest interest for the vehicle technology program. The reviewer stated that the combination of scanning transmission electron microscopy/electron energy loss spectroscopy (STEM/EELS), X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS) and first principle computations is a powerful approach to understanding the structure of important materials as well as understanding the effect of structure on properties such as voltage fade and material instability. The reviewer observed that the main work to date has been on cobalt containing lithium manganese rich materials. Future work will involve similar studies to understand the structure of silicon lithium alloys.

Reviewer 3:

The reviewer commented that if a material is an insulator such as LiFePO₄, then the conduction band information is irrelevant. The reviewer further added that the drawing was not making sense. The reviewer inquired about simply stating, "empty DOS near the Fermi level."



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.**Reviewer 1:**

The reviewer commented that the PI did a lot of work and presented many results. However, the reviewer said that it was difficult from the presentation to adequately review the PI's results and conclusions. As indicated, many of these results will be published, and the reviewer looked forward to reading about them.

Reviewer 2:

This reviewer indicated that the migration of manganese and nickel ions to the lithium layer was discovered in the presence of oxygen vacancies. This can result in the formation of spinel material and voltage fade. The reviewer went on to say that the substitution of cobalt had beneficial effects on voltage fade. The reviewer added that morphology control also had beneficial effects on voltage fade.

Reviewer 3:

This person stated that tossing in nice-looking drawings and images do not mean much. The reviewer asked what material had been studied in the achievement, and asked about high voltage spinel. The reviewer commented that there was not much explanation or captions on figures. The reviewer asked if the PI was expecting the reader to read all of the cited literature.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer observed that the PI had several collaborations and found it a little surprising that the PI did not have more collaborations, considering the breadth of what the PI had studied.

Reviewer 2:

The reviewer asked what data was contributed and by who, and what the partners' was. The reviewer wanted to know what the difference was between "collaborators" and "partners" after having noted a difference in the listing.

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.**Reviewer 1:**

The reviewer said that the future work indicates that the PI is finishing up the cathode studies and moving on to Si. The reviewer said that it would be interesting to see what recommendations the PI suggests for an improved high energy cathode material.

Reviewer 2:

The reviewer said that the effect of coatings will be important because of sensitivity of methods to surface will make it more easily studied.

Reviewer 3:

The reviewer commented that unlike the title, no ion transport data was present although the project had been going on more than a year. The reviewer then wanted to know when the data/calculations concerning ion transport in the materials are gathered.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer said that the PI does not make a great case for relevance, but that the materials studied were very important to advanced lithium-ion battery technologies.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

This reviewer was not sure about the resources, but noted that there were many names listed.

Reviewer 2:

This reviewer was not sure how the PI had the resources to conduct these studies in sufficient depth.

Daikin Advanced Lithium Ion Battery Technology - High Voltage Electrolyte: Ron Hendershot (Daikin America) - es217

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer said that the project was well-designed and feasible to tackle the technical barriers. The literature review and baseline development are comprehensive. The reviewer then recommended that for electrochemical window evaluation, together with platinum, carbon (e.g., glass carbon) should be considered as well.

Reviewer 2:

This reviewer said that the approach seemed to be good. However, the reviewer suggested that the authors have to make sure that the supply of raw material is reliable and consistent, since this could be particularly critical when dealing with battery materials.

Reviewer 3:

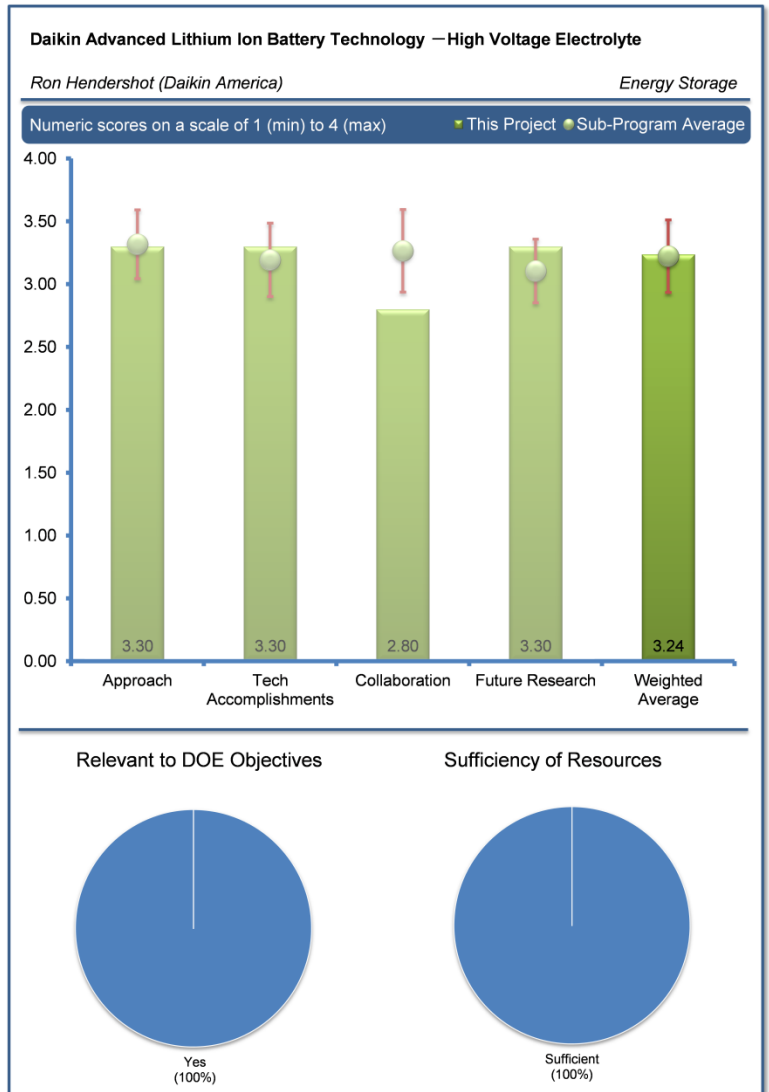
The reviewer said that the study started in October 2013, and had made reasonable progress in developing a R&D program. The reviewer continued to note that a listing of high voltage electrolyte materials, conductivity, viscosity stable voltage range, etc. had been compiled. A list of electrolyte additives/solvents, their properties and their supplier had been developed. Further, the reviewer commented that the identification of promising high voltage electrolytes had started. The study is at a very early stage and experimental work is a learning experience.

Reviewer 4:

The reviewer reiterated that the objective of the project is to develop an electrolyte that can cycle up to 5 volts and is safe (self-extinguishing). To meet this goal, the program focuses on identifying electrolytes containing fluorocarbons for improved SEI layers. The reviewer added that the project addresses some of the key technical barriers confronting lithium battery technology.

Reviewer 5:

The reviewers pointed out that the researchers used the design of experiments approach which is in the very early stage; and needs to see what parameters and at how many levels are being assessed to better understand the scope. The reviewer added that it was important to provide cost estimates for the baseline versus newly developed formulations to have at least an understanding of the value proposition and, thus, probability of the commercial success.



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.**Reviewer 1:**

This reviewer commented that the project had just started and that the authors have shown good progress.

Reviewer 2:

This reviewer stated that the project was on the right track. The technical achievement contributed to the understanding the performance of various electrolytes for high voltage application.

Reviewer 3:

This reviewer recounted that the project was initiated in October 2013. During this 6-month time frame (i.e., October - April), satisfactory progress was achieved. A comprehensive review of electrolytes was conducted that included a review of Daikin's internal data and external literature. As a result of these studies, two electrolytes were selected as baseline formulations. The electrolytes were analyzed in terms of conductivity, voltage window stability and temperature stability. Electrolytes were also evaluated in cells. The reviewer concluded that the results are promising. Preliminary data show an increase in capacity retention when cells are charged to 4.6V.

Reviewer 4:

This reviewer said that it was too early to assess the progress and accomplishments of the project; however the initial results looked promising.

Reviewer 5:

This reviewer stated that the characteristic basic elements for developing new cell high performance components that have been identified had been obtained. The reviewer added that voltage stability range and conductivities had been obtained.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer noted that there would be collaborations with Coulometrics, LLC who would be helping with cell fabrication and testing. The reviewer added that it would be beneficial for the program and for the PI to be in communication with other VTO laboratories. This would be helpful in terms of electrode fabrication and to ensure cell testing methods are valid.

Reviewer 2:

This reviewer noted that the program was in its early stages, and further reported that Voltammetry has developed the stable range of common solvents and other properties of conductivity. A simple differential scanning calorimetry (DSC) testing was confirmed to supply safety data of electrolyte behavior in a cell. The reviewer observed that baseline properties had been collected.

Reviewer 3:

This reviewer commented that the project had just started and commented that additional collaborations should be encouraged.

Reviewer 4:

This reviewer said that the PI should make an effort to collaborate outside the organization, especially academic institutions, to further understand the mechanism for the performance of the electrolytes observed.

Reviewer 5:

This reviewer stated that the characterization of the SEI layer might require establishing collaborations with the universities/national laboratories, unless the company has internal capabilities.

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.

Reviewer 1:

This reviewer noted that the plan for future works covered the ground of the interested area, but that the PI should extend the scope to investigate new potential active material in the electrolytes.

Reviewer 2:

This reviewer commented that the program plan had been developed and work had begun. To date, the reviewer observed that the progress was typical.

Reviewer 3:

This reviewer commented that the future efforts were appropriate. Efforts will begin on characterizing the SEI layer formed by the additives. Cells (NMC/graphite and LMN/graphite) containing the various electrolyte formulations will be built and tested. The reviewer added that cells would be evaluated when charged at high voltages.

Reviewer 4:

This reviewer stated that it was not clear in which type of cell the authors would be testing the two baseline electrolytes. Also, that the physical surface analysis for the SEI formation was not clearly specified.

Reviewer 5:

The reviewer said that the future work was well aligned with the project objectives. The reviewer noted that there was not enough data yet to provide recommendations. This reviewer continued to say that it might be beneficial to use commercially available electrode materials for the baseline comparison.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer commented that the project does support the overall DOE goals. Electrolyte investigation is critical for the development of high energy Li or Li-ion batteries for transportation technologies.

Reviewer 2:

This reviewer said noted that the effort is relevant and supports DOE's objective of petroleum displacement. The project is attempting to identify high voltage electrolytes that could result in higher energy density batteries.

Reviewer 3:

This reviewer indicated that the data collected and interpreted would be valuable.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

This reviewer assumed that the company has a good instrumentation base for characterization of the SEI additives (surface analysis).

Reviewer 2:

This reviewer commented that sufficient resources were available to carry out the project.

Reviewer 3:

At this time in the project, the reviewer said that the level of resources appeared to be sufficient.

Reviewer 4:

The reviewer said that the PI seems to have adequate resources for the work. However, the reviewer encouraged the PIs to extend their collaboration outside the organization.

Fluorinated Electrolyte for 5-V Li-Ion Chemistry: John Zhang (Argonne National Laboratory) - es218

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer commented that the goal of this project is to develop advanced electrolyte materials that can significantly improve electrochemical performance without sacrificing the safety of the lithium-ion battery. The reviewer recounted that the project would pay attention to affordability. To do this, the project will develop electrolyte materials that can tolerate voltages greater than 5V. High voltage electrolyte candidates will be screened with the aid of quantum chemistry modeling and electrochemical methods. The electrolytes will include fluorinated carbonates and they will be evaluated using $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO)/LTO and LNMO/graphite chemistries. According to this reviewer, this approach is excellent.

Reviewer 2:

The reviewer commented that the project had a well-designed approach that tackled the barriers.

Reviewer 3:

The reviewer said that with the aid of quantum calculations, promising compounds for 5V electrolytes were designed/identified, synthesized, characterized and evaluated. These are necessary to use the high voltage cathode materials under development. The goal is to use molecular engineering to identify promising compounds and verify their stability by experimentation.

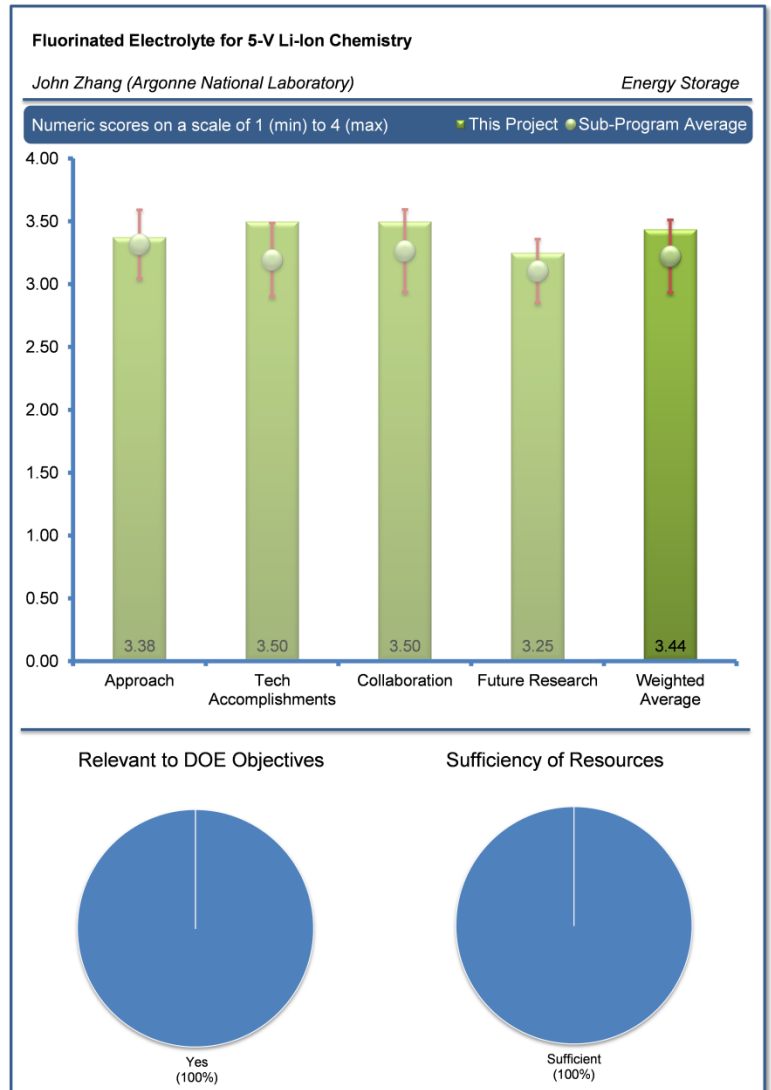
Reviewer 4:

It seemed to this reviewer that the PI's approach's for the project was to use modeling to provide guidance for the synthesis, than to test the new electrolyte in cell. It appears that the fluorinated compounds demonstrated the performance improvement, but the theoretical base for the molecule design was not quite clear. The electrochemical testing was not complete, e.g. cyclic voltammetry ought to be used to identify the electrochemical window (should be used to verify the calculated HOMO/LUMO), AC impedance and fitting should be used as well; besides SEM, more structural analysis should be done on the SEI layers.

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.

Reviewer 1:

The reviewer noted that excellent progress had been made since this project was initiated in October 2013.



Reviewer 2:

The reviewer said that the performance of the synthesis electrolyte demonstrated superior performance than control electrolyte. The PI should expand the scope of testing to variable cathode/anode materials.

Reviewer 3:

The reviewer noted that the authors already reported significant results for a fairly new project.

Reviewer 4:

The reviewer commented that the initial experimentation has begun. The reviewer observed that some electrolytes are not stable at higher voltages. There is a relationship between the electronic structure of the electrolyte molecules and their stability.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer commented that the use of molecular engineering principles (DFT, etc.) is a giant step in the right direction. Today molecular calculations are proving useful in a number of areas. It is fitting to adopt this into identifying high voltage battery materials as well as stability.

Reviewer 2:

The reviewer indicated that the potential for good collaboration with other institutions appeared to be in place. The institutions include: the U.S. Army Research Laboratory (collaborator), Brookhaven National Laboratory (BNL) (collaborator), University of Rhode Island (interaction), Jet Propulsion Laboratory (interaction), and Dr. Larry Curtiss – Theoretical modeling.

Reviewer 3:

The reviewer said that the PI's collaboration with other national laboratories is important and fruitful.

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.**Reviewer 1:**

This reviewer thought that the proposed future research was reasonable and well thought-out. During the remainder of FY 2014 the project would continue to explore the additive effect on the newly developed high-voltage fluorinated electrolyte (HVE) 1 on the graphite electrode. Efforts will continue to design and synthesize new fluorinated carbonate solvents based on the recent research results. In addition, tailored cathode electrolyte interphase (CEI) additives will be employed to further improve the stability of the LNMO/electrolyte interphase.

Reviewer 2:

The reviewer commented that using the rest of 2014 to explore and identify new compounds is very much in order. Once a base is established the project should be able to make significant contributions and speed the development of high voltage systems needed for the future demands.

Reviewer 3:

The reviewer stated that it is always difficult to know if the authors are going to succeed; but that the theoretical approach coupled with organic synthesis and in-situ measurements is highly encouraging.

Reviewer 4:

The reviewer suggested that the PI should allocate more resources to the advance analysis especially in-situ diagnostics for the SEI formation and to focus more attentions on the development of additives and conduct adequate electrochemical analysis beyond simple coin cell charge and discharge.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This reviewer said that the project was highly relevant and supports the overall DOE objective of petroleum displacement. To replace petroleum, a high energy density battery must be developed, and a high voltage electrolyte would be one approach to achieve this.

Reviewer 2:

The reviewer noted that the development of high voltage electrolyte contributes to the overall goal of DOE.

Reviewer 3:

This reviewer said that calculations can take the place of trial and error. Designer electrolytes, cathodes and anodes are very much in order for the future.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

This reviewer said that the present resources were adequate. Once a pattern of success is realized, then additional funding will be in order.

Reviewer 2:

The reviewer indicated that the resources were sufficient to complete this effort.

Reviewer 3:

This reviewer stated that the PI had adequate resources for the investigation, but that the lead PI should allocate the resources more smartly.

Novel Non-Carbonate Based Electrolytes for Silicon Anodes: Dee Strand (Wildcat Discovery) - es219

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

This reviewer said that the high throughput approach was excellent for the initial screening. Based on the discussion during the poster session, experiments were conducted in duplicates. The reviewer commented that there was no data suggesting how reproducible the results are. The focus on the 3M specific cell chemistry narrows the scope to one design. It might be important to do some benchmarking testing of the selected formulations

Reviewer 2:

The reviewer commented that the approach was clear, well-reasoned, systematic, and addressed one of the key technical barriers of lithium ion batteries. Non-carbonate electrolytes will be developed such that they can form stable SEIs on a 3M silicon alloy anode, have comparable ionic conductivity to carbonate formulations, are oxidatively stable to 4.6V, and will not increase cell cost. Silicon anodes will be investigated because it holds the promise of significantly improving energy density.

Reviewer 3:

This reviewer stated that the final use of 18650 cells is important. The reviewer suggested that the authors should be careful and make sure the materials received for testing are of similar quality since this is very important, particularly when talking about battery materials.

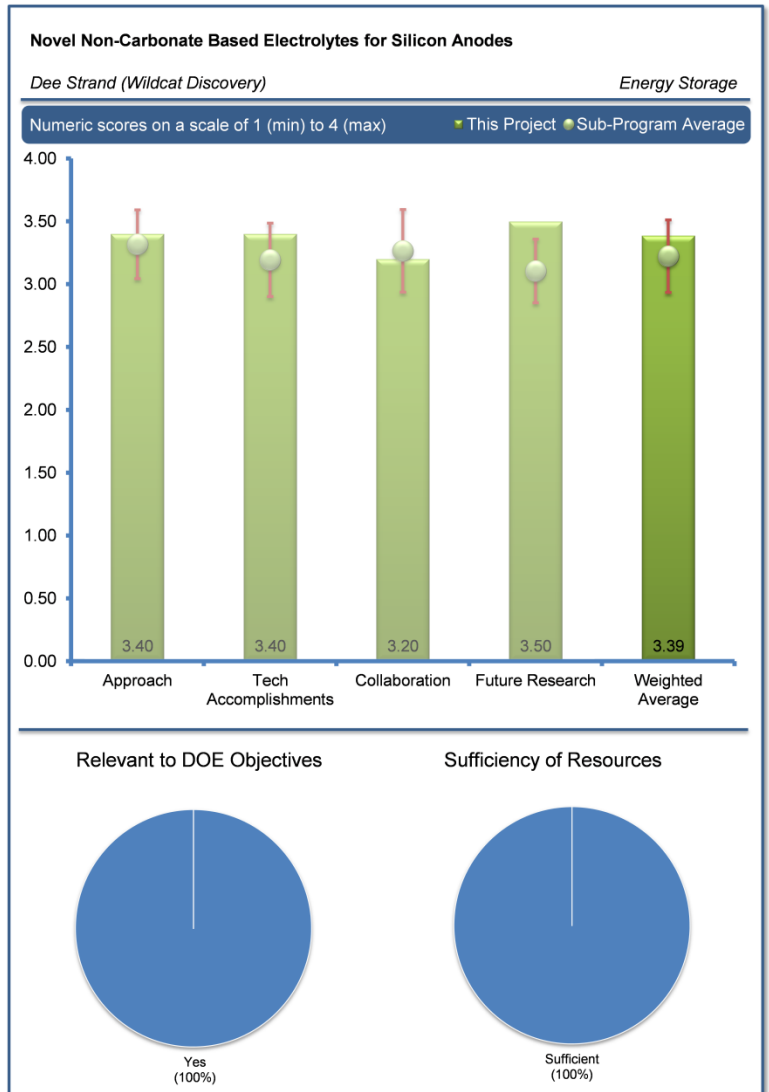
Reviewer 4:

The reviewer said that the PI screened a large amount of alternatives against the benchmark electrolyte. The approach for the screening, recounted the reviewer, is to use first capacity, first cycle efficiency and either the 50th or 75th capacity retention. Although those are valid quick engineering evaluations, the reviewer recommended that the PI conduct some electrochemical or physical testing for the electrodes, so that the evaluation could be more focused.

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.

Reviewer 1:

The reviewer indicated that good progress had been made in a relatively short period of time. Eighty two electrolytes were tested, some of which look very promising.



Reviewer 2:

This reviewer said that an impressive amount of work was conducted in a short period of time. The reviewer added that it would be helpful to have inserts/separate graphs for the promising/selected formulations vs. control; the reviewer clarified that the data was somewhat cluttered.

Reviewer 3:

The reviewer said that the project was on-track to achieve the milestones. With about 85 different electrolyte combination screens, the potential winner indeed surfaced. However, due to lack of in-depth electrochemical and physical analysis, the reviewer noted that little guidance was provided from the existing work regarding future development.

Reviewer 4:

The reviewer stated that the project is relatively new. Surface analysis of the SEI should be pursued at some point. This is an interesting approach where the silicon anodes should be able to play a critical role.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

This reviewer observed that there will be some collaborations/interactions with 3M but that it was not clear to what extent.

Reviewer 2:

This reviewer stated that it appeared that the only partner was the only beneficiary of this project. Thus, the reviewer suggested establishing collaboration with other companies within the BATT program to understand the applicability of the findings and to study SEI formation.

Reviewer 3:

This reviewer stated that further collaboration with other groups was strongly encouraged.

Reviewer 4:

This reviewer noted that the objective was to develop an electrolyte for the 3M silicon anode and that the collaboration with 3M was critical. The reviewer then recommended that the PI take more advantage of UCSD's analysis capability of materials.

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.**Reviewer 1:**

This reviewer said that the plan for the future work was well design. More electrochemical analysis (e.g., AC impedance) should be beneficial for the understanding.

Reviewer 2:

This reviewer stated that this was a very well-planned program.

Reviewer 3:

This reviewer noted that testing and collaboration with 3M was important and added that it was also important to have some intimate knowledge about how the 18650 cells are fabricated and to be able to follow and analyze the data as it is produced.

Reviewer 4:

The reviewer commented that the proposed future plans were appropriate and well-reasoned. Efforts will continue to identify non-carbonate solvents as well as a polymer additive for improved SEI layer formation.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This reviewer stated that this project was highly relevant and supports DOE's objectives to displace petroleum with electric drive systems. For example, the EV Everywhere battery goals for 2022 are a cost of \$125/kWh and energy densities of 400 Wh/L and 250 Wh/kg. This will require higher energy density systems and new electrolytes and additives that help the battery cycle will be of immense benefit.

Reviewer 2:

The reviewer said that the development of adequate electrolyte for the Si anode will contribute to the performance improvement of the Li batteries, which is suitable for the department goal.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer stated that sufficient resources appeared to be in place at this time.

Reviewer 2:

The reviewer commented that the PI had adequate resources for the project, which should be better utilized.

Predicting Microstructure and Performance for Optimal Cell Fabrication: Dean Wheeler (Brigham Young University) - es220

Reviewer Sample Size

A total of six reviewers evaluated this project.

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.

Reviewer 1:

The reviewer thought that this approach was absolutely outstanding. The reviewer continued to say that it was elegant, well characterized, and that the PIs had done an excellent job of validating their approach.

Reviewer 2:

This reviewer said that this was very innovative work very and that it was much needed for the quality control and electrode design improvements.

Reviewer 3:

The reviewer commented that the development of this new technique of measuring the electronic (and hopefully soon, the ionic) conductivity of composite electrodes is quite significant and could add substantially to the tools available to the battery designer. The reviewer would like to see the method extended to measurements as a function of formulation as well as processing parameters such as calendaring pressure, coating speed and temperature, etc. This would help in developing and optimizing electrode manufacture to the extent that it is within the scope of the contract. Finally, the reviewer would have liked to see cell tests done on cells with electrodes of the same material and electrolyte, but different electronic/ionic conductivity due to processing conditions or formulation.

Reviewer 4:

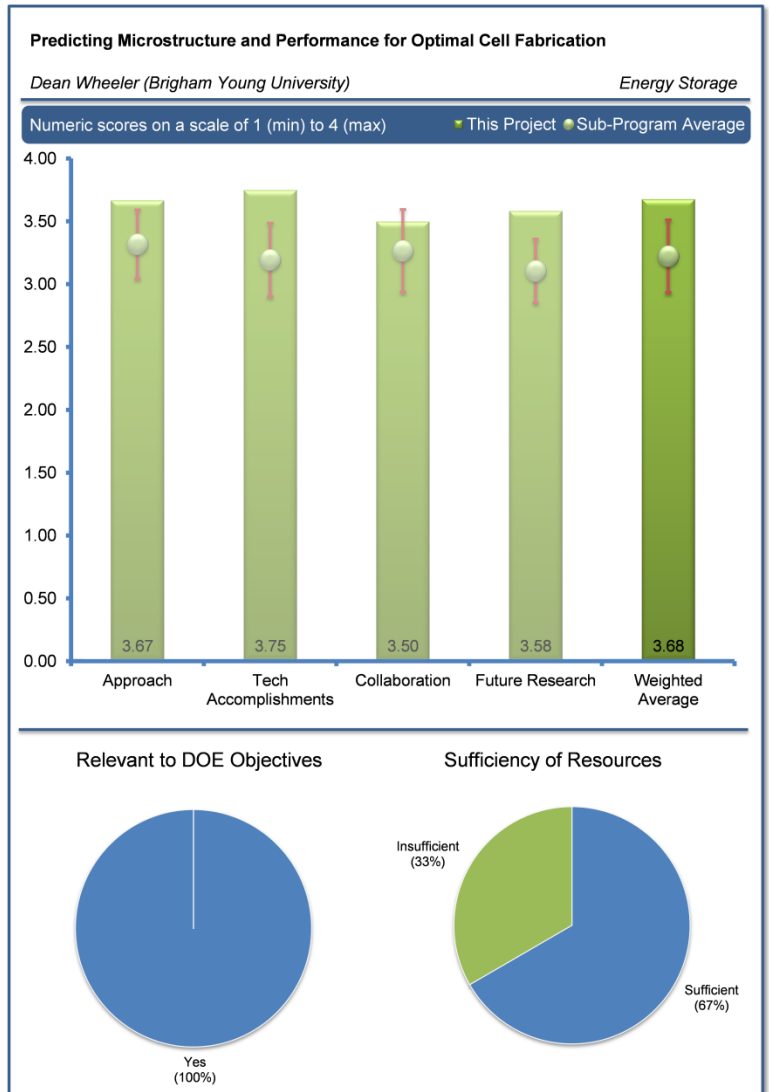
The reviewer stated that the project was well designed and that it was already showing interesting results.

Reviewer 5:

The reviewer commented that the PIs focus on electronic conductivity effects in electrodes. This tends to be more important for cathodes where the active materials are generally poor conductors. The reviewer remarked the PIs overall plan was good. However, the more challenging aspects of the project are left for the later years.

Reviewer 6:

The reviewer stated that the PIs completed the development of the first generation of multi-probe devices for conductivity measurements and that the probes were validated. Clearly, the milestones were met and the approach is valid. The reviewer then suggested that the PI address the electrode active materials particle size issues that would occur in the same order of the distances between the probes. Thus, continued this reviewer, there would be evaluation of how the boundary effect was being considered.



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.**Reviewer 1:**

The reviewer stated that the proven success was that the industry partner was acquiring the technology. The reviewer thought there was a very honest assessment of the results and implications and commended the project on an excellent execution.

Reviewer 2:

This reviewer commented on how it has always been hard to measure the conductivity of a thin film of semiconductor material on a conductive carrier – the problem is how much of the current between the probes goes through the electrode material and how much through the carrier. The reviewer then commended that this group had successfully produced a tool that could measure both conductivity within a thin film and also the contact resistance of that film to the carrier in a relatively simple manner. As far as the reviewer knew, there was no way to measure either of these with any accuracy. Moreover, the reviewer said the project demonstrated both excellent accuracy (using standards) and really quite surprising repeatability. According to the reviewer, the project had a wide range of conductivity on a typical electrode material, which was surprising. Work like this could really help improve electrode uniformity and ensure even current distribution of cells under high rates of charge and discharge. The reviewer continued to say that this was the best method poster/talk the reviewer had seen at the AMR or any other recent meeting and represented a clear advance in the state of the art of battery technology for Li-ion and other battery systems.

Reviewer 3:

This reviewer said that even though this project was relatively new, the authors have shown great progress.

Reviewer 4:

This reviewer noted that the progress in developing the technique was substantial. However, the presentation did not delineate the sources of error in the measurement, and this would have been useful in evaluating the method.

Reviewer 5:

The reviewer said that the progress of the project was satisfactory. The research would make an impact on electrode manufacture, especially quality control.

Reviewer 6:

The reviewer stated that the PI developed a technique to easily measure conductivity and current collector contact resistance in a finished laminate, which had not been done previously. It extends the classical four probe measuring technique to a dimension smaller than the thickness of the electrode for the measurement to be made. This technique should be able to be effectively transferred to industry.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer observed that the communication with A123 and national laboratory personnel was good. It would be even more useful to be able to specify variations in formulation and processing conditions as discussed above, so that automated electrode manufacture could be applied to reveal these effects more precisely.

Reviewer 2:

The reviewer thought that the project was getting lots of interest from the industry.

Reviewer 3:

The reviewer acknowledged that the PI had established many collaborations in academia, industry, and with the national laboratories.

Reviewer 4:

The reviewer noted that the PIs closely collaborated with battery manufacturers (e.g., A123 Systems), which gave the PI a real-world production perspective.

Reviewer 5:

The reviewer strongly encouraged collaboration with additional institutions.

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.

Reviewer 1:

The reviewer commented that the future work plan was well designed and added that the PI should add electrode particle size and porosity into consideration and compare them against the conductivity data.

Reviewer 2:

This reviewer said that this was a very practical and important quality manufacturing technique. This technique may end up reducing the amount of off spec material in a production facility.

Reviewer 3:

The reviewer stated that the PI had a good plan going forward. His work on modeling the coating process should prove interesting.

Reviewer 4:

The reviewer stated that the microstructure model may be more difficult to achieve the desired accuracy than the PI hoped for. It is certainly worth the effort to develop such a model, however, as it could add an additional dimension to the largely empirical process of electrode manufacture design as used presently.

Reviewer 5:

The reviewer was looking at spatial variation of conductivity. The reviewer observed that the project also plans to add an electrolyte and to try to measure the ionic conductivity of an electrode film as well, which would again be extremely valuable. The reviewer thinks that knowledge like this would be invaluable inputs to cell designers and especially to modelers. The reviewer suggested that it might be good to compare their spatial mapping of electrode conductivity with thermal images of the electrodes hit by a heat pulse to see if they match (thinking heat conduction and electronic conduction often go hand in hand).

Reviewer 6:

The reviewer said that it was very important to validate the technique using same active materials fabricated into the electrodes by different suppliers. The reviewer asked if this technique could be used for quality control, in particular to spot metallic particles in the electrode. This would be very important to ensure safety of the Li-ion batteries. If possible, the reviewer commented that this work should be given a highest priority.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

The reviewer said that the PI made a solid case for relevance.

Reviewer 2:

The reviewer said that this method actually addresses two key issues associated with thin electrodes used for many battery systems, Li-Ion, primary lithium, air cells, etc. The fact that the project could for the first time get “real” conductivity in such films is enormously important to the battery industry.

Reviewer 3:

The reviewer said that the project research on the 3D profile of the conductivity of porous electrode would provide a valuable tool for the electrode production, improve quality control and cutting the production cost, which contribute the overall goal of DOE.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

Based on the PI's productivity, there seemed to be sufficient funds to conduct the studies.

Reviewer 2:

The reviewer said that the PI had adequate resources for the investigation.

Reviewer 3:

This reviewer would like this work expanded to provide a clear way for others, in and outside the DOE's programs, to build and use devices based on their work. The reviewer said that the project had created an industry-wide asset that needs to be widely disseminated and leveraged.

A Combined Experimental and Modeling Approach for the Design of High Coulombic Efficiency Si Electrodes: Xingcheng Xiao (General Motors LLC) - es221

Reviewer Sample Size

A total of three reviewers evaluated this project.

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.

Reviewer 1:

The reviewer said that the combination of modeling and experiment approaches were very effective to verify each other and that the group successfully achieved that.

Reviewer 2:

The reviewer said that the PI had put together an impressive group to examine and attack the mechanical issues on silicon alloy electrodes. The effort included extensive experimental and theoretical studies.

Reviewer 3:

The reviewer stated that the approach was not clearly delineated. However, to the extent that the reviewer understood the effort, it appeared to be proceeding as designed. The reviewer stated that the comparison of uncoated silicon and core shell silicon to yolk-shell silicon seemed contrived. It would be better in the reviewer's opinion to show comparisons to the best available samples from the literature.

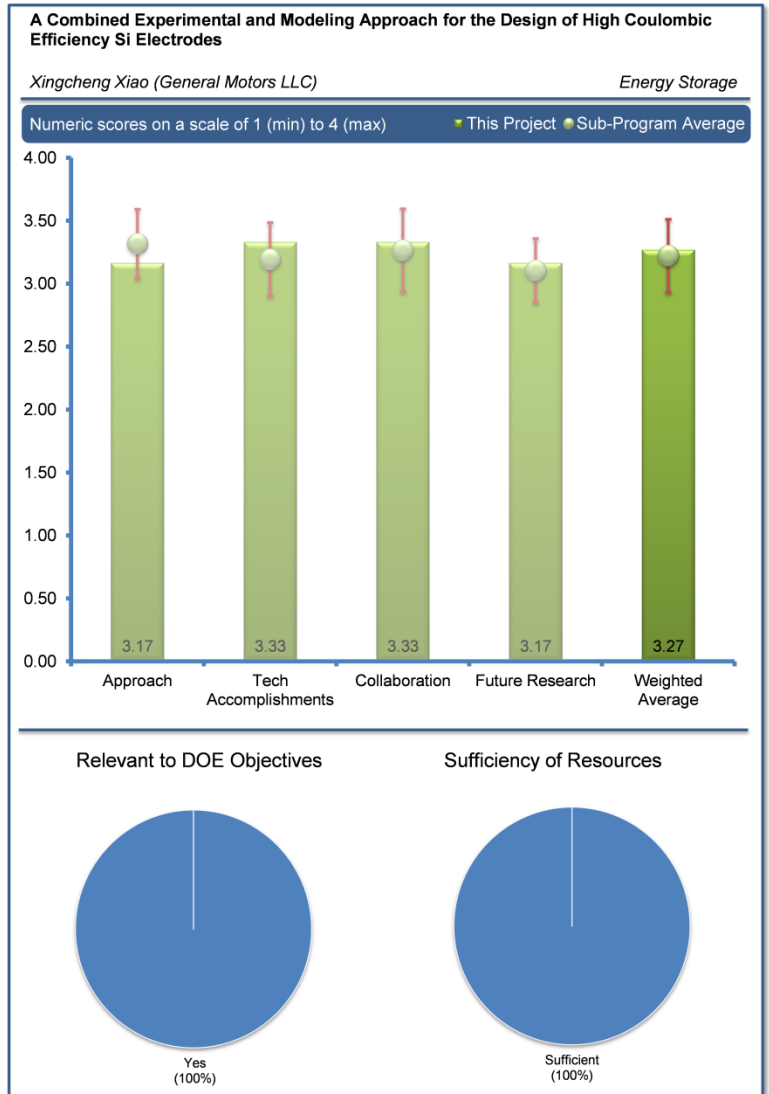
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer said that the PI had a broad spectrum of results that clearly demonstrated that the project had been very productive and is off to a great start.

Reviewer 2:

The reviewer said that the project has acquired high quality data for better understanding. In particular, relating the cell height changes to the in situ microscopic data on shelled Si particles is outstanding for obtaining insight into the material dynamics subjected to electrochemical processes. On the other hand, the interpretation of Al₂O₃ ALD data (accomplishment 2) is questionable because the shell can be partial when it is less than 10 atomic layers.



Reviewer 3:

The reviewer said that the milestones already completed indicated that some real progress had been made in trying to understand the effects of coatings. However, it would be useful to show the uniformity and repeatability of the ALD coatings in order to better assess the measurements. Also, some attempt to determine the accuracy of the measurements would be useful.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer said that this group had a great research network.

Reviewer 2:

The reviewer said that the PI had a number of collaborations.

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.

Reviewer 1:

The reviewer said that it would be interesting to follow this project as it moves forward.

Reviewer 2:

The reviewer described the proposed future research as too physical, and added that some characterizations of the chemical nature of materials are recommended through collaborations.

Reviewer 3:

The reviewer said that the relevance would be improved with better attention to accuracy and uniformity of materials and coatings.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer said that the PI made a good case for relevance.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer said that it was hard to see how the funds supported the level of effort.

Electrode Architecture-Assembly of Battery Materials and Electrodes: Karim Zaghib (Hydro Quebec) - es222

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer pointed out that the overall approach was excellent in meeting the project objectives. To be more effective, it might be beneficial for Headquarters to utilize knowledge and findings within the BATT program instead of developing new Si anodes and electrode formulations. This way more time could be allocated to developing low cost electrode architectures with good electrochemical performance. This will allow to best utilize the HQ' strengths and to avoid overlapping with the work done by others within the BATT program.

Reviewer 2:

The reviewer stated that the electrode architecture by controlling tortuosity and porosity and maintaining high ionic conductivity is a good approach.

Reviewer 3:

This reviewer stated that this was a very important contribution to high capacity cells using a new generation of anodes. The reviewer added that there were very interesting in-situ results provided by SEM.

Reviewer 4:

The reviewer said that the project approach was effective to identify the major issues associated with the Si anode, and analyze the cause for those problems.

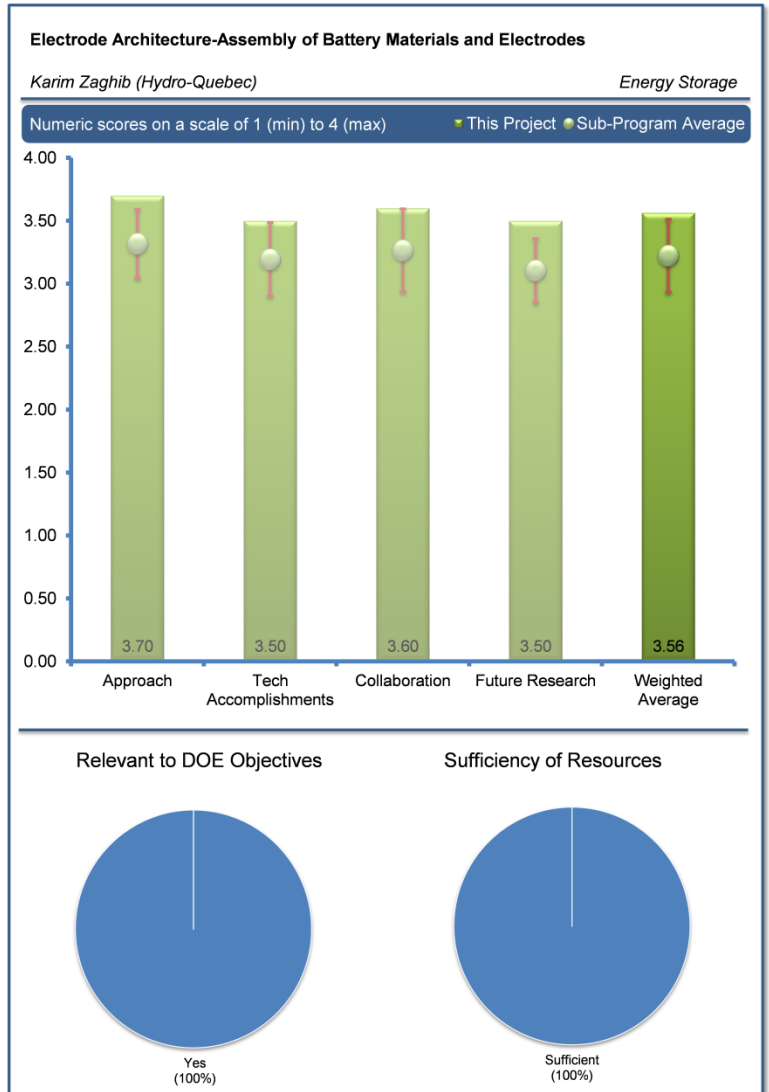
Reviewer 5:

This reviewer said that this project addressed technical barriers by designing Si electrode architecture for improved lithium ion battery energy density. In-situ and ex-situ characterization techniques are used to investigate SEI.

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.

Reviewer 1:

The reviewer observed that the work done to date was solid and confirmed industry knowledge. The reviewer added that it was important for HQ to take leadership in providing direction towards commercial approaches.



Reviewer 2:

The reviewer said that important results were already provided in a fairly new project.

Reviewer 3:

This reviewer observed that Si anode was one of the DOE focus areas. The results from the project shine light to the root cause of the problem with Si anode, and the possible ways to alleviate those problems by engineering electrode structure design.

Reviewer 4:

This reviewer observed that this project had identified Si-based anode with a capacity of 1200mAh/g and provided Si power to other BATT PIs. However, the charge/discharge efficiency at deep discharge status is still a challenge which may affect battery cycle life.

Reviewer 5:

This reviewer commented that the loading of silicon should be given.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer commented that this project brought together some excellent research from various different institutions to attack the technical barriers together.

Reviewer 2:

The reviewer stated that there was good collaboration.

Reviewer 3:

The reviewer indicated that the PI collaborated with both an academic institution and a national laboratory effectively.

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.**Reviewer 1:**

The reviewer said that future activities were in-line with achieving project goals.

Reviewer 2:

The reviewer noted that the future activities were well aligned with the deliverables, but that it was not clear what the critical assumptions and issues were.

Reviewer 3:

The reviewer recounted that interesting results were already reported. The high carbon content for these Si anodes seemed to be a good compromise that may overcome the electrode degradation.

Reviewer 4:

The reviewer said that future activities were in-line with achieving project goals.

Reviewer 5:

The reviewer noted that the future activities were well aligned with the deliverables, but that it was not clear what the critical assumptions and issues were.

Reviewer 6:

The reviewer said that the proposed future research was reasonable as planned.

Reviewer 7:

This reviewer commented that the loading of the silicon for the current experiment as well as for the proposed future experiment should be given.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer commented that the goals of this project were highly relevant to DOE targets to increase battery energy density and cycle life.

Reviewer 2:

The reviewer commented that the engineering development for the Si anode process was in-line with overall goal of DOE.

Reviewer 3:

This reviewer noted that the project reduces the petroleum use.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

To this reviewer, it appeared that the PI had sufficient resources to conduct the proposed work.

Reviewer 2:

This reviewer commented that there were sufficient resources.

Reviewer 3:

The reviewer noted that the PI had adequate resources for the investigation.

Advanced Binder for Electrode Materials: Gao Liu (Lawrence Berkeley National Laboratory) - es223

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer said that the functional conductive polymer binder approach was very good.

Reviewer 2:

The reviewer stated that the PI developed a unique conductive and elastic binder which is used in a rechargeable Si anode for Li-ion batteries. The conductive binder can compensate the volume change during the Si anode cycling, and therefore maintain the integrity of the Si anode. The reviewer continued to say that the approach to solve the cyclability problem for Si anode was sound.

Reviewer 3:

This reviewer said that the project had a very interesting approach to the Si anode. The use of conductive polymers, together with spherical Si, may be the right approach to improve the stability of these new type of electrodes.

Reviewer 4:

This reviewer said that the project targets the improvement of Si-based anode insufficient energy density and poor cycle life for lithium ion battery applications.

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.

Reviewer 1:

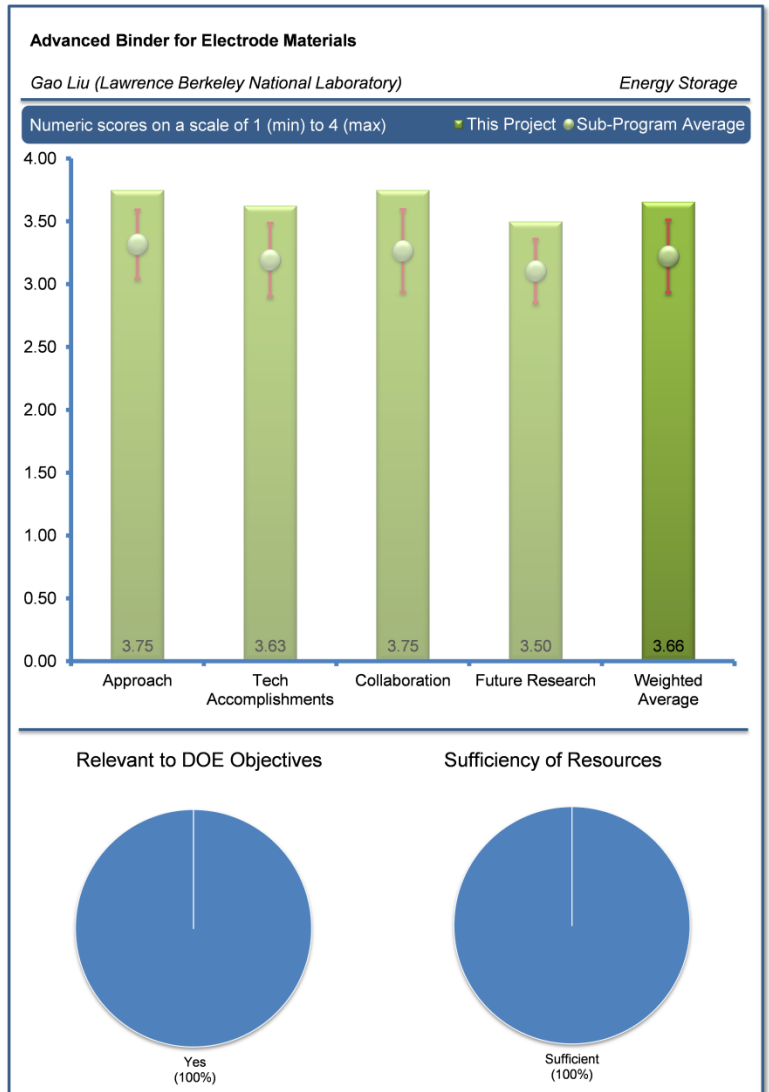
The reviewer commented that the performance was very good with conducting binder approach. The reviewer wanted to know what the current loading was.

Reviewer 2:

The reviewer noted that there was great progress for a fairly new project.

Reviewer 3:

The reviewer said that improved performance had been demonstrated. The project is on track and all the milestones were met.



Reviewer 4:

This reviewer said that the project had achieved many progress in terms of conducting binders and Si-based anode material. However, recycling efficiency and life seemed to still be challenges ahead.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer stated that the PI had excellent collaboration with researchers from different institutions to attack the technical barriers together.

Reviewer 2:

The reviewer commented that there was excellent collaboration.

Reviewer 3:

The reviewer said that the PI formed a strong collaboration with various national laboratories and industries.

Reviewer 4:

The reviewer noticed that several teams were collaborating.

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.

Reviewer 1:

The reviewer stated that the 3 mAh/cm² loading was a good target. The reviewer added that a postmortem analysis was important.

Reviewer 2:

The reviewer said that the proposed future research was well planned and feasible. The PI should focus its attentions on the elastic SEI formation.

Reviewer 3:

The reviewer noted that the project was on schedule and that the proposed future work was reasonable. The reviewer was not sure if this project had a go/no-go plan. If not, a go/no-go plan may be needed or illustrated in the review slides for project planning purpose.

Reviewer 4:

The reviewer said that it was not clear which type of cells the authors would be using to validate their best anode design. Is the reviewer strongly recommended to use cylindrical or pouch cells.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer commented that the project supported the DOE objectives and that it targeted attacking Si-based anode technical barriers for improved battery life and energy density.

Reviewer 2:

The reviewer stated that the project aimed to alleviate the problem associated with the rechargeable Si anode, which is in line with the DOE goal.

Reviewer 3:

The reviewer said that the project reduces petroleum use.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

This reviewer said that there were sufficient resources.

Reviewer 2:

This reviewer said that it appeared that there were sufficient resources for this project to achieve the goals described.

Reviewer 3:

The reviewer said that the PI had adequate resources to accomplish the tasks.

Fundamental Studies of Lithium-Sulfur Cell Chemistry: Nitash Balsara (Lawrence Berkeley National Laboratory) - es224

Reviewer Sample Size

A total of five reviewers evaluated this project.

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.

Reviewer 1:

The reviewer noted that the project aims to identify the polysulfide species using X-ray absorption techniques and calculation. The approach to tackle the problem is sound.

Reviewer 2:

The reviewer commented that the project had an interesting theoretical approach linked to experimental results. The study of the sulfur (S) chemistry should be one of the critical areas that can move forward the lithium-sulfur (Li-S) cells.

Reviewer 3:

This reviewer said that the work was focused on the fundamental understanding of the sulfur cathodes products and includes the experimental validation steps. The reviewer added that it might be beneficial to benchmark even initial findings vs. results reported in the literature.

Reviewer 4:

The reviewer said that if the high energy density benefit of the Li-S battery is to be realized, then there must be a fundamental understanding of the polysulfides that limits its performance. This effort will provide a fundamental science-based understanding of the redox reaction products (polysulfides). It will enable rational cell design strategies. First-principles molecular dynamics simulations will be used to determine charge distribution and X-ray absorption spectra of polysulfide solutions will be used to help in the identification of the various species. Finally the reviewer concluded that this method would allow a simple hypothesis for sulfur oxidation in ether-based solvents to be obtained.

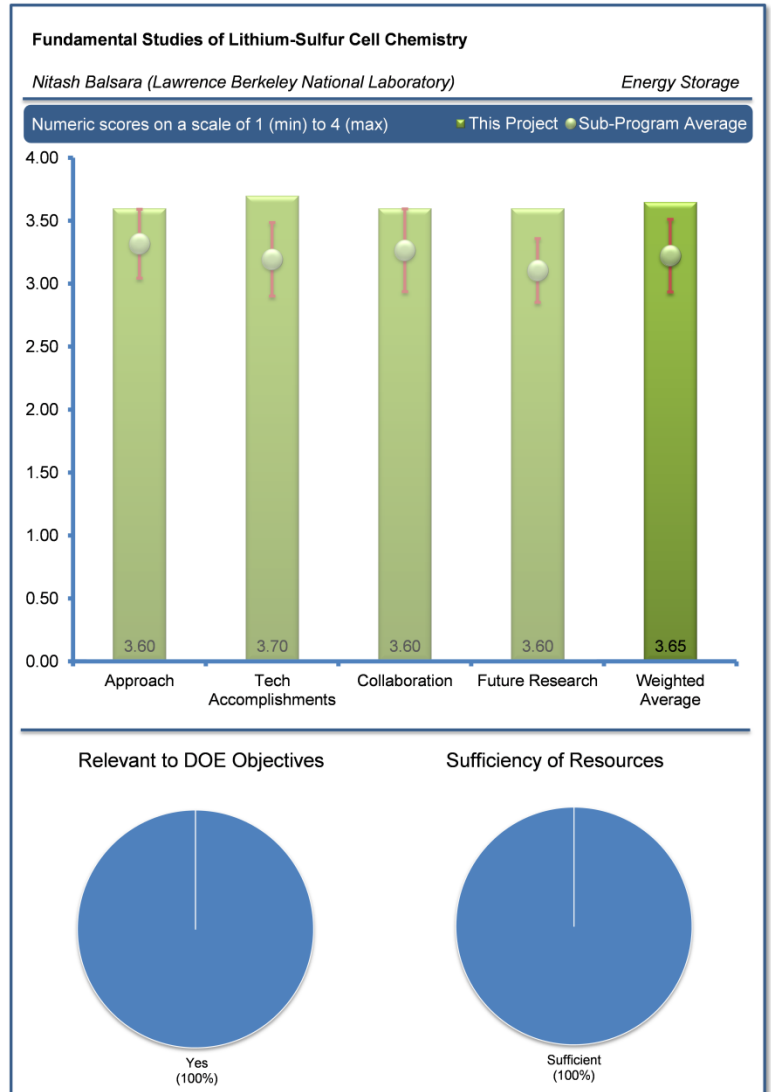
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

The reviewer noted that the PI had found a unique way to transform the liquid polysulfide ions into a solid polymer, therefore the X-ray analysis could be conducted. The reviewer observed that the ternary diagrams were established and thought the project was progressing well.

Reviewer 2:

The reviewer commented that the project had demonstrated significant progress. The project has shown that only Li_2S_4 and Li_2S_8 species were likely to exist in the sulfur cathode during cycling.



Reviewer 3:

The reviewer said that for a fairly new project, the results shown by the authors were encouraging.

Reviewer 4:

The reviewer noted that the use of principal component analysis (PCA) seemed to provide unbiased conclusions on the components in the S cathode. The reviewer was looking forward to seeing experimental data.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer observed that an appropriate level of collaboration existed. These include National Energy Research Scientific Computing Center (NERSC), ALS, LBNL, University of Illinois, ONRL and BNL. The reviewer added that many of the investigators were within the Vehicle Technology Office and that this was very good.

Reviewer 2:

The reviewer said that the PI collaborated with researchers in another national laboratory and academic institution. The reviewer continued to say that such collaboration was suitable for the project.

Reviewer 3:

This reviewer stated that correlating results of statistical modeling vs. data reported in the literature is important for the validation of the use of the PCA. The reviewer added that the project needs to establish more collaboration with leading research groups.

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.**Reviewer 1:**

The reviewer stated that the proposed future efforts were appropriate and were clearly defined. It is an excellent idea to perform in situ experiments to create polysulfides by electrochemical reactions and then to use fingerprinting strategy to determine reaction products.

Reviewer 2:

The reviewer noted that there were very well articulated future plans.

Reviewer 3:

The reviewer indicated that the future work for the continuous X-ray experiments was sound. The reviewer added that other analytical technics should be used to validate the results alongside with X-ray absorption.

Reviewer 4:

The reviewer stated that in-situ measurements to study reaction products, and design simulation to better understand the sulfur cathode may end up moving this field forward.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

This reviewer observed that the project aimed to understand polysulfide ions, which was critical for the development of Li-S batteries.

Reviewer 2:

To this reviewer, obtaining a fundamental knowledge of the polysulfide reaction products in a lithium sulfur battery is highly relevant. This supports DOE objective of petroleum displacement.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

The reviewer noted that the PI had adequate resources to accomplish the tasks.

Reviewer 2:

The reviewer commented that the resources were sufficient for this project.

Design and Synthesis of Advanced High-Energy Cathode Materials: Guoying Chen (Lawrence Berkeley National Laboratory) - es225

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

This approach, the reviewer fully approved of. The program could use this powerful experimental tool to overcome the barriers between the experimentalist and the mathematician. The reviewer proceeded to say that both need each other but often feel challenged by their presence.

Reviewer 2:

The reviewer stated that the project has addressed one of important problem for all high voltage cathode materials which is stability.

Reviewer 3:

The reviewer summarized that the project objective is to obtain a fundamental understanding on the phase transition mechanisms, kinetic barriers, and cyclic instabilities (as a function of crystallographic planes) in high-energy cathode materials. The commenter explained that the approach adopted is to use single-crystal model systems and to perform advanced ex-situ and in-situ studies to characterize the crystal-plan specific transport properties and interfacial chemistry. Based on these studies, the reviewer noted that direct correlations between crystal structure, composition, morphology, performance, and stability will be established, which will help in the design of optimized high-performance electrode materials. The project evaluator agreed that this approach is consistent with the objectives of this project as well as the goals of the DOE ABR program, is well-integrated with the other materials-based efforts, and appears to be feasible.

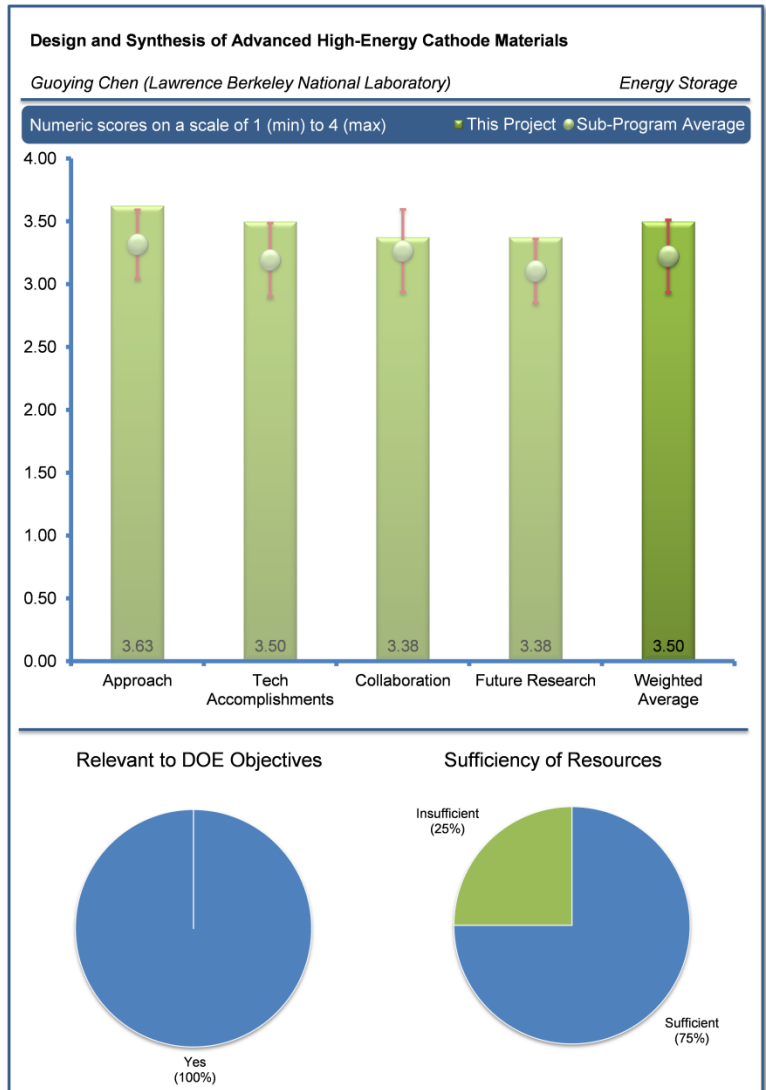
Reviewer 4:

The reviewer commented that the approach taken combining single crystals, as well as diagnostic and modeling studies in the project, are yielding results helpful for improved synthesis of high capacity cathode materials and better understanding of their fade mechanisms.

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.

Reviewer 1:

The reviewer noted that there was a rich collection of quite interesting data that was still not enough to pinpoint the key criteria for improved synthesis of the cathode materials but the reviewer was hopeful that the remaining tasks would go a long way toward achieving that goal.



Reviewer 2:

The reviewer applauded that impressive studies were made that led to a good understanding on the effects of crystallographic planes on the interfacial stability. The commenter also explained that single crystals of high-voltage LMNO and layered oxide cathodes were synthesized with a variety of sizes and morphologies and studied for self-discharge, interfacial stability and cycle life. It was shown clearly that the side reactions and self-discharge are reduced on the 111 plane compared to 112 plane of the LMNO cathode and that the electrode performance could be manipulated by particle morphology engineering. The reviewer noted that similar single crystal studies have been carried out to understand the effect of morphology and particle size on the activation kinetics and interfacial stability of layered oxides. The commenter stated that these results are quite interesting, but cautioned that then one would ask the relevance of this understanding from a single-crystal behavior in a polycrystalline electrode, i.e., if we one control the crystalline facets of the cathode. The project evaluator asked whether it would it be possible to synthesize bulk materials with the desired crystalline facets. The commenter also noted that good characterization tests are underway on these single crystal cathodes, including Li_xMNO solid solutions. Overall, the reviewer acknowledged that good progress has been demonstrated towards the DOE goals.

Reviewer 3:

The reviewer stated that hopefully, the experimentalists can realize the need for cooperation is making a success for the program for electrification of the transportation in the United States. The reviewer continued to say that each could make rapid progress if there was cooperation. This reviewer further explained that it really is a combination of experimentalist and quantum calculation to more accurately identify promising, new high energy materials. The reviewer pointed out that there is a need to keep both sides happy.

Reviewer 4:

The reviewer observed that the research has been focused on the comparison of two different kinds of single crystals: plane versus octahedron single crystals. The chemical and electrochemical stabilities have been investigated. The crystallinity and surface states during aging had also been investigated.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

The reviewer observed that there were a great team of collaborators.

Reviewer 2:

The reviewer stated that there are excellent on-going collaborations with researchers from LBNL and from universities.

Reviewer 3:

This reviewer said that the collaboration appeared to be appreciated.

Reviewer 4:

The reviewer commented that there were limited outside collaborative activities, except with ANL for the particle mapping.

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.**Reviewer 1:**

The reviewer observed that the proposed future research focused on understanding phase transition mechanisms, kinetic barriers, and instabilities of high voltage cathode.

Reviewer 2:

The reviewer summarized that the proposed future research is to continue further evaluation of the impact of surface properties, including surface modifications, on side reaction kinetics and products as well as capacity fade in high-voltage cathode materials and to explore other aspects of particle engineering to improve cathode performance and stability. The single-particle diagnostic studies will be extended to the layered-layered oxides to understand their structural changes and voltage fade and impedance growth upon cycling. The

commenter also described that the studies will focus on constructing the LxMNO phase diagram to establish solid solution versus two-phase behavior, and thus understand the stability and performance of these materials as functions of Li content and temperature. The commenter agreed that the proposed studies are logical, while addressing the technology barriers, so are consistent with the DOE goals.

Reviewer 3:

This reviewer commented to learn as you go, and that it will take time for both sides to accept the other and create a really powerful team. The reviewer continued that the human mind is a marvelous organ, and to have an assist to carry out the new concepts would be outstanding.

Reviewer 4:

The reviewer said that of course, issues such as capacity and voltage fades were key targets of studies. Additional studies at the particle level should include severe gassing at the outset. The reviewer then asked about TM dissolution studies.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?**Reviewer 1:**

The reviewer noted that this approach was the wave of the future. The reviewer encouraged to keep it going.

Reviewer 2:

This reviewer said that extremely focused studies to improve synthesis of high energy cathode materials is key to developing a long-life, low-cost battery for vehicle propulsion.

Reviewer 3:

This reviewer stated to develop high-capacity high voltage cathode for Li-ion batteries.

Reviewer 4:

The reviewer highlighted that the limited driving range and higher cost of the Li-ion batteries are serious impediments for their use in electric vehicles. The commenter explained that high energy density electrode materials will result in improved specific energy for Li-ion cells, increased driving range for the vehicle, as well as reduced overall cost for the battery. The state-of-the-art cathode materials provide capacities of only ~160 mAh/g, which are about half of the capacities possible from the carbon anodes. The reviewer confirmed that the battery research community needs to develop new cathode materials, based on basic understanding of these materials, as is being addressed by this project.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?**Reviewer 1:**

The reviewer proposed increasing the funds for such a high-powered group.

Reviewer 2:

The reviewer said that the resources are adequate for the scope of the project.

Reviewer 3:

The reviewer said that for now, resources were adequate.

Microscopy Investigation on the Fading Mechanism of Electrode Materials: Chongmin Wang (Pacific Northwest National Laboratory) - es226

Reviewer Sample Size

A total of four reviewers evaluated this project.

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.

Reviewer 1:

The reviewer said that it was good to see the atomic level dynamics. However, the information obtained may be too local to make strong connection with the ensemble behavior of particles in the electrochemical condition that contains highly convolved surfaces, interfaces, crystalline faces, etc.

Reviewer 2:

The reviewer said that the PI proposes to use TEM, EELS, and EDS to study advanced electrode materials. The reviewer added that the use of in situ cells made this work more interesting.

Reviewer 3:

This reviewer observed that the project had an interesting and innovative approach to try and get some in situ measurements of battery electrodes and their interfaces.

Reviewer 4:

The reviewer commented that the development of in-situ method of studying active materials during electrochemical changes could yield important information about the mechanisms for degradation reactions as well as structural changes occurring during the cycling of the material.

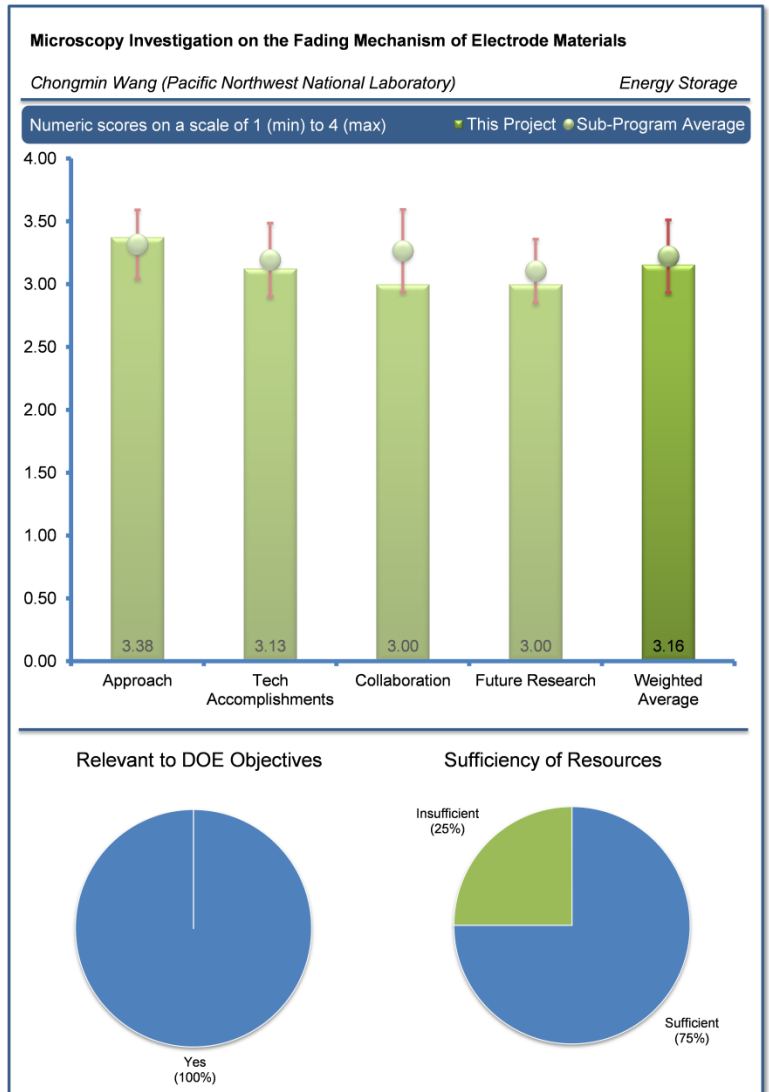
Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:

According to this reviewer, the project’s accomplishments and progress seemed to be going well. The reviewer thought that there was nice in situ TEM work. Then the reviewer added that it would be good if the method could be used to study the SEI formation in terms of organic species from the electrolyte; the reviewer was not sure if this was really possible with the window used.

Reviewer 2:

The reviewer commented that the development of the operando TEM liquid electrolyte cell is a real step forward. The studies of lithiated silicon coated with conductive polymer and the lithium manganese rich cathode material are good demonstrations of the technique. The reviewer would have liked to see better definition of the materials studied in future presentations, however. The specific conductive



polymer is quite important to the operation of the electrode, but no definition of the polymer used is given. Also, the reviewer added that the physical parameters of the cathode material are quite important to function.

Reviewer 3:

The reviewer said that the PI had conducted many microscopy studies on both advanced anode and cathode materials and electrodes. The reviewer especially liked the in-situ cell development.

Reviewer 4:

This reviewer noted that the Si is wrapped with conductive polymer, and wanted to know what the volumetric capacity was. The reviewer then commented that the TEM images showed that a very small fraction was Si (Slide 7). The reviewer continued to say that the correlation between Ni segregation with capacity fading in the Li excess materials was good. The EDS image on crack formation did not support that atom segregation is responsible and asked if the two were related.

Question 3: Collaboration and coordination with other institutions.**Reviewer 1:**

This reviewer observed that the collaborations were well established.

Reviewer 2:

This reviewer said that the collaboration and coordination with other institutions looked good.

Reviewer 3:

The reviewer said that the PI had established many collaborations.

Reviewer 4:

This reviewer stated that this was more of a stand-alone method development project, but it would seem to overlap a bit with some of the X-Ray techniques being used by BNL to study surface and bulk electrode compositions. The reviewer then suggested maybe talking to BNL, if it has not already been done.

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.

Reviewer 1:

This reviewer observed that the plans for things to study looked fine.

Reviewer 2:

The reviewer observed that the PI proposed more diagnostic studies and added that it would be interesting to see what guidance the PI gave on improving the electrode materials.

Reviewer 3:

This reviewer suggested considering benchmarking with other materials.

Reviewer 4:

This reviewer would have liked to see an emphasis on solving real problems with the technique such as voltage fade in lithium manganese rich materials and inefficiency if cycling lithiated silicon.

Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

Reviewer 1:

According to this reviewer, this project could become a very useful tool in addressing fundamental studies of electrode interfaces and electrode/electrolyte reactions.

Reviewer 2:

The reviewer discussed that the PI's choice of electrode materials studied made this project relevant.

Question 6: Resources: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

This reviewer was not sure how the project was being conducted on the stated funds.

Acronyms and Abbreviations

Acronym	Definition
3D	Three Dimensional
ABR	Advanced Battery Research
AC	Alternating current
Ah	Ampere-hour
ALD	Atomic Layer Deposition
AMR	Annual Merit Review
ANL	Argonne National Laboratory
ARK	Abuse Reaction Kinetics
ARL	Army Research Lab
ATR	Attenuated Total Reflectance
BATT	Batteries for Advanced Transportation Technologies
BMS	Battery Management System
BNL	Brookhaven National Laboratory
C	Carbon
CAD	Computer-aided design
CAE	Computer-aided engineering
CAEBAT	Computer-aided engineering of batteries
CAMP	Cell Analysis, Modeling, and Prototyping
CATARC	China Automotive Technology and Research Center
CEI	Cathode electrolyte interphase
CMC	Carboxymethyl Cellulose
CNT	Carbon Nanotubes
Co	Cobalt
Cr	Chromium
CSTR	Continually stirred tank reactor
Cu	Copper
DEDOHC	Dioxohexane dicarboxylate
DFT	Density Functional Theory
DOE	Department of Energy
DSC	Differential Scanning Calorimetry
EC	Ethylene Carbonate
ECT	Electrochemical-Thermal Coupling
EDS	Energy Dispersive X-ray Spectroscopy
EELS	Electron Energy Loss Spectroscopy
EIS	Electrochemical Impedance Spectroscopy
EPR	Electron Paramagnetic Resonance
EV	Electric Vehicle
EXAFS	Extended X-ray Absorption Fine Structure
F	Fluorine
FCG	Full concentration gradient
Fe	Iron

Acronym	Definition
FEC	Fluorinated ethylene carbonate
FTIR	Fourier Transform Infrared Spectroscopy
FY	Fiscal Year
GM	General Motors
HCMR	High capacity manganese rich
HEV	Hybrid Electric Vehicle
HR	High-resolution
HRSXRD	High-resolution Synchrotron X-ray Diffraction
HRTEM	high-resolution transmission electron microscopy
HVE	High-voltage fluorinated electrolyte
HVM	High-volume Manufacturing
IE	Ion exchange
INL	Idaho National Laboratory
IR	Infrared
JCI	Johnson Controls, Inc.
LBNL	Lawrence Berkeley National Laboratory
LCO	Lithium Cobalt Oxide
LEESS	Lower-Energy Energy Storage System
LFO	Lithium Iron Oxide
LFP	Lithium Iron Phosphate
Li	Lithium
Li₂MnO₃	Lithiated transition metal oxides
LIB	Lithium Ion Battery
LiBF₄	Lithium tetrafluoroborate
LiBOB	Lithium bis(oxalato)borate
LIBS	Laser-induced breakdown spectroscopy
Li-ion	Lithium Ion
LiPF₆	Effective electrolyte salt for lithium-ion battery
LiPON	Lithium Phosphorous Oxynitride
LiTFSI	Lithium Bis(Trifluoromethanesulfonyl)Imide
LL	Layered lithium
LLC	Layered-layered spinel composite
LMNO	Ni-substituted manganese spinel oxides
LMO	Lithium Manganese Oxide
LMR	Lithium Manganese Rich
LT	Low Temperature
Mg	Magnesium
MIT	Massachusetts institute of Technology
Mn	Manganese
NaOH	Sodium hydroxide
NCA	Battery cathode material (nickel cobalt aluminum oxide)
NCM	Nickel Cobalt Manganese
NERSC	National Energy Research Scientific Computing Center

Acronym	Definition
NDE	Non-Destructive Evaluation
Ni	Nickel
NMC	Nickel Manganese Cobalt oxide
NMP	N-Methylpyrrolidone
NMR	Nuclear Magnetic Resonance
NP	Nail penetration
NREL	National Renewable Energy Laboratory
O₂	Oxygen
OAS	Open architecture standard
ORNL	Oak Ridge National Laboratory
P	Phosphorous
PAN	Polyacrylonitrile
PCA	Principal component analysis
PEV	Plug-in Electric Vehicle
PHEV	Plug-In Hybrid Electric Vehicle
PI	Principal Investigator
PRC	People's Republic of China
PVDF	Polyvinylidene difluoride
QC	Quality Control
R&D	Research and Development
ROM	Reduced-Order Models
Ru	Ruthenium
S	Sulfur
Sb	Antimony
SEI	Solid Electrolyte Interface
SEM	Scanning Electron Microscope
SFG	Sum frequency generation
Si	Silicon
Sn	Tin
SNL	Sandia National Laboratory
SOC	State of Charge
STEM	Scanning transmission electron microscopy
TEM	Transmission Electron Microscope
Ti	Titanium
TM	Transition Metal
TMA	Tri Methyl Aluminum
TXM	Transmission x-ray microscope
USABC	US Advanced Battery Consortium
USCAR	U.S. Council for Automotive Research
V	Volts
VC	Vinylene Carbonate
VTO	Vehicle Technology Office
XANES	X-ray Absorption Near Edge Spectroscopy

Acronym	Definition
XAS	X-ray Absorption Spectroscopy
XPS	X-ray Photoelectron Spectroscopy
XRD	X-ray Diffraction (Crystallography)
XRF	X-ray Fluorescence